Solitons and production of defects in flow-aligning nematic liquid crystals under simple shear flow

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Abstract The production of defects in flow-aligning nematic liquid crystals under simple shear flow is analyzed by linear stability analysis based on Leslie-Ericksen theory. It is pointed out that the equation of motion of the nematic director under simple shear flow conforms to the driven over-damped sine-Gordon equation and has a soliton solution of amplitude \( \pi \). It has also been shown that the stationary state with the director uniformly oriented at a Leslie angle is only a metastable state and that the potential which governs the motion of the director has infinite numbers of stable stationary states. Therefore the defects appearing as a stable solitary solution can be nucleated from a uniformly aligned flow-aligning type of nematic liquid crystal by shear flow. On the other hand the bands with long axis parallel to the vorticity axis appearing as an unstable solution can be observed as transient patterns at low shear rate and low shear strain value. The theoretical predictions are compared with previous experimental observations.

Keywords nematic liquid crystals, defects, solitons.

In recent years an extensively studied example is a homeotropically aligned nematic liquid crystal in a continuously rotating magnetic field\textsuperscript{1} 1\textsuperscript{1} to 5\textsuperscript{1}. In this example due to the coupling between director gradient and fluid flow many kinds of soliton patterns such as defect lines\textsuperscript{12} concentric rings\textsuperscript{13} \& \textsuperscript{14} lattices of concentric rings\textsuperscript{15} \& \textsuperscript{16} and spirals\textsuperscript{17} \& \textsuperscript{18} have been observed experimentally. The mechanisms and the onset conditions for these soliton structures have been theoretically analyzed\textsuperscript{19} \& \textsuperscript{20}.

Another interesting example is the instability of the director field in a homeotropically aligned nematic liquid crystal subjected to elliptical shear flow\textsuperscript{21} \& \textsuperscript{22}. In this case roll structures are observed due to the interaction between convective rolls and the director distortion.

It was also discovered many years ago that there are two types of nematic liquid crystals flow-aligning and flow-tumbling nematic. Here tumbling refers to continual rotation of the director with time and aligning means that in the steady state the director adopts an orientation of zero-viscous torque within the shearing plane and close to the flow direction. The flow behavior of liquid crystals has been summarized in several review articles\textsuperscript{23} 7\textsuperscript{2} to 10\textsuperscript{2}.

Many transient and stationary patterns are observed during and after the cessation of shear flow. In the following we adopt the terminology widely used in literature for describing the patterns. Roll-cells with the roll axis parallel to the flow direction are called stripes\textsuperscript{24} the periodic band texture with the band axis parallel to the vorticity axis is called bands. Under shear flow\textsuperscript{25} stripes\textsuperscript{26} roll cells\textsuperscript{27} are found experimentally for many polymeric nematic liquid crystals\textsuperscript{28} 11\textsuperscript{29}. It is generally believed that the stripes only exist in tumbling type nematics or in the tumbling regime of polymeric nematic liquid crystals. Linear stability analysis has been applied to the appearance of stripes\textsuperscript{29} and the structure and the onset condition for the roll cells have been given\textsuperscript{30}. Band and thread textures are also found during shear\textsuperscript{31} \& \textsuperscript{32} especially when the shear rate and/or the shear strain are low\textsuperscript{33} 15\textsuperscript{34}. On the other hand after cessation of shear flow\textsuperscript{35} the pattern observed experimentally is usually the band structure\textsuperscript{11} 37\textsuperscript{36} 38\textsuperscript{37}.

It is generally believed that nematics of the tum-
bling type should be candidates for defect production because of their propensity for various flow instabilities \cite{19}. Indeed, optical observations during shear flow have shown the production of defects \cite{20}. For the flow-aligning nematics, the general belief is that when a shear flow starts, the director tends to align in the flow direction with an angle \( \theta \) called Leslie angle \cite{21}. Tilted away from the flow direction. In fact, the situation is not as simple as expected. Surprisingly, it is found that in initially aligned samples of typical flow-aligning type low molecular weight nematic liquid crystals such as 5CB \cite{19}, plenty of defects are also produced during shear flow. These findings make the connection between tumbling and defect production unclear and they have introduced an uncertainty in assigning the flow-aligning and flow-tumbling type of nematic liquid crystals. At least, defect production during shear cannot be simply viewed as the signal of the onset of director tumbling or director wagging.

However, the most crucial questions are the following: i) is the shear-induced defect production an intrinsic property of the flow-aligning type of liquid crystals? In other words, is the state with the director uniformly aligned along the Leslie angle stable for a shear-aligning type of nematic liquid crystal? ii) if the uniformly aligned state is not stable, what are the mechanisms and the onset conditions for the appearance of spatially non-uniform structures?

1 Stability of uniform stationary states

The geometry of the experiment is a slab of a nematic liquid crystal of thickness \( d \) confined between two parallel glass plates. The simple shear flow has the flow velocity \( v \) in the \( x \) direction and the velocity gradient direction in the \( y \) direction \cite{22}. \( v_y = \gamma y \) where \( \gamma \) is the shear rate. The schematic drawing of the geometry of the system is shown in Fig. 1. For simplicity, the director \( \mathbf{n} \) is confined in the \( x-y \) plane and can be described by the angle \( \theta \) measured from the \( y \)-axis. This is a good approximation for the shear-aligning type of nematic liquid crystals.

Since we are only interested in the spatial structure in the velocity gradient direction \cite{23} it is assumed that the system is uniform in the \( x \) direction \cite{24}. i.e. the spatial inhomogeneity occurs only in the \( y \) direction. By taking into account the balance between the viscous torque and the elastic torque that act on the director while neglecting the back-flow effect and the inertial term, the equation of motion of the director under single elastic constant approximation and the one-dimensional approximation can be written as

\[
\gamma_1 \frac{\partial \theta}{\partial t} = K \frac{\partial^2 \theta}{\partial y^2} + \mu_3 \sin^2 \theta - \mu_2 \cos^2 \theta \gamma. \] 1
\]

Here \( K \) is the Frank’s elastic constant \cite{25} \( \mu_2 \) and \( \mu_3 \) are two Leslie coefficients \cite{26} and \( \gamma_1 = \mu_3 - \mu_2 \) is the rotation or twist viscosity. The rotation viscosity must be positive \cite{27} therefore the constraint \( \gamma_1 = \mu_3 - \mu_2 > 0 \) should be satisfied. When the sample thickness \( d \) is much larger than the boundary layer of the cell \cite{28}, the one-dimensional approximation holds true.

We should note in advance that Eq.1 can also be written as

\[
K \frac{\partial^2 \theta}{\partial y^2} - \gamma_1 \frac{\partial \theta}{\partial t} + \frac{1}{2} \mu_3 - \mu_2 \gamma \]

\[
- \frac{1}{2} \mu_3 + \mu_2 \gamma \cos 2 \theta = 0 \] 2

which conforms to the driven over-damped sine-Gordon equation \cite{29}

\[
\kappa \frac{\partial^2 \theta}{\partial y^2} - \gamma \frac{\partial \theta}{\partial t} + F - V_0 \sin \theta = 0 \] 3

where \( V_0 \) is the maximum potential and \( F \) the driving force. It has been found that the driven over-damped sine-Gordon equation has a solution of stable propagating soliton of amplitude 2 \cite{30}. Eq.2 also conforms to the equation for describing the experiment of rotating magnetic field with the back-flow effect neglected \cite{31}. Therefore, one can easily expect that complex spatial structures could exist in flow-aligning nematics under shear flow. When \( \gamma y \ll c \) the velocity of the soliton \( \partial \theta / \partial t + \gamma y \partial \theta / \partial x \approx \partial \theta / \partial x \) is true. So we can also obtain the same results in the \( x \) direction.

We first discuss the dynamics of a uniform system which is described by Eq.1 without the spatial derivatives.
\[ \gamma_1 \frac{\partial \theta}{\partial t} = \Delta \mu_3 \sin^2 \theta - \mu_2 \cos^2 \theta \frac{\partial \theta}{\partial \phi}. \]

Eq. (3) reveals that there exist two kinds of solutions, i.e., shear-aligning and -tumbling. For a system with \( \mu_2 \mu_3 > 0 \), the shear-aligning type solution can be found. Thus we call it shear-aligning system.

For the non-stationary state, i.e., \( \mu_2 \mu_3 < 0 \), Eq. (3) has to be described by time-dependent director motion of a uniform system. Actually, Eq. (3) can be analytically solved in the cases with or without external magnetic field \( \Delta \mu \). Both theoretical analysis \( \Delta \mu \) and Brownian dynamics simulations \( \Delta \mu \) found that in the non-stationary state the director is continuously rotating with time with a well-defined time period. However, in this work we will focus on the case of a shear-aligning system which has \( \mu_2 \mu_3 > 0 \) i.e., both \( \mu_2 \) and \( \mu_3 \) have the same signs.

In the shear-aligning system there exist two stationary solutions:

\[ \theta_{\Omega} = k \pi + \arctan \left( \pm \frac{\mu_2}{\mu_3} \right). \]

In the above equation the subscripts \( s \) and \( u \) stand for stable and unstable. The stability of the stationary states can be assigned by linear stability analysis which leads to the results that for a system with both \( \mu_2 \mu_3 < 0 \)

\[ \theta_s = k \pi + \arctan \left( \frac{\sqrt{\mu_2}}{\mu_3} \right) \]

\[ \theta_u = k \pi + \arctan \left( -\frac{\sqrt{\mu_2}}{\mu_3} \right) = k \pi - \arctan \left( \frac{\mu_2}{\mu_3} \right). \]

If both \( \mu_2 \mu_3 > 0 \) the stability of the above solutions is reversed. In the next section we will see that the so-called stable stationary states are only metastable.

2 Spatial inhomogeneity

Taking account of the spatial inhomogeneity, Eq. (1) or (2) should be used. In order to analyze the possibility of structure and the conditions for the onset of spatial structures the strategy of Ref. (22) will be closely followed.

2.1 Potential energy

The motion of the director described by Eq. (2) can also be written as

\[ \gamma_1 \frac{\partial \theta}{\partial t} = \frac{\partial \theta}{\partial \phi}. \]

In the above equation the energy functional which governs the director motion is written as

\[ \theta (\theta) = \int d \phi \left( \theta \theta + \frac{\partial \frac{\partial \theta}{\partial \phi}}{\partial \phi} \right) \]

with the potential energy density

\[ \theta (\theta) = - \frac{1}{2} \mu_2 \mu_3 \theta + \frac{1}{2} \mu_3 \mu_2 \sin 2 \theta. \]

The potential energy density \( \theta (\theta) \) has the stationary points. In order to see this more clearly the plots of \( \theta (\theta) \) are given in Fig. 2 and \( \theta_s \) and \( \theta_u \) are labeled. In the following numerical calculations we set \( \mu_2 = -0.4 \) and \( \mu_3 = -0.04 \) which corresponds to the values of 5CB at a temperature of 32°C.

The potential energy densities corresponding to the stable and unstable stationary states are \( \theta_s \) and \( \theta_u \) respectively. Correspondingly the energy density difference between the stable and unstable stationary states \( \Delta V \) which is corresponding to the energy barrier for the system transform from a stable stationary state to the next unstable stationary state is written as

\[ \Delta V = \theta (\theta) - \theta (\theta) \]

\[ = - \int d \phi \left( \pm \mu_3 - \mu_2 \theta + \frac{\pi}{2} \pm \arctan \left( \frac{\mu_2}{\mu_3} \right) \right. \]

\[ \pm \sqrt{\mu_2 \mu_3} \int \phi \]

where the upper sign is for the system in which both \( \mu_2 \) and \( \mu_3 \) are negative and the lower sign is for the system in which both \( \mu_2 \) and \( \mu_3 \) are positive. We should mention that the energy barrier for the system of \( \theta_{\Omega k} \) to climb up to the next hill of \( \theta_{\Omega k + 1} \) and transform to the next minimum of \( \theta_{\Omega k + 1} \) is low when the shear rate is low. Therefore the thermal

![Fig. 2. The potential \( \theta (\theta) \) for \( \gamma = 5 \) s\(^{-1}\) and \( \gamma = 10 \) s\(^{-1}\) with \( \mu_2 = -0.4 \mu_3 = -0.04 \).](image)
fluctuation and the mechanical noises introduced by shear flow should be able to lead the system to sequentially transform to the lower valleys. We should also mention that the height of the barrier \( \Delta V \) increases with an increase in shear rate.

From Fig. 2 it is seen that if the director is aligned in the stationary state of \( \theta_{\text{cr}} \) the potential of state \( k \) is higher than that of the state \( k + 1 \) i.e. \( \theta_{\text{cr}} + 1 = \theta_{\text{cr}} + \pi \). Due to the fact that the potential \( V \theta \) has infinite stationary states there can exist states in which \( \theta \) increases monotonically undergoing more or less discrete changes \( \pi \) at each pair of defect. Although we know that the nematic liquid crystals have the property of \( \mathbf{n} = - \mathbf{n} \) and the energy should be the same if all the nematic liquid crystalline molecules have rotated an angle of \( \pi \) here the potential energy \( \mathbb{V} \theta \) simply tells us that the states of certain \( \theta_{\text{cr}} k = 0 \) 1 2 \ldots \) are only metastable states and thus the fluctuation-assisted transition of the system from one minimum to the next one will be most likely to occur through a time sequence of configurations requiring the minimum intermediate elevation in energy. If one block of the directors in the middle of the system is rotated by an angle of \( \pi \) i.e. it has been transformed into the stationary state of \( \theta_{\text{cr}} + 1 \) while all the others are staying in the stationary state of \( \theta_{\text{cr}} \) then one pair of defects are generated. We should mention here that the term of defect is widely used in the literature of liquid crystals and it is termed kink and anti-kink by Buttiker and Landauer \( ^{210} \) or in the literature of condensed state physics \( ^{270} \). The fact is that the block that has rotated an angle of \( \pi \) has gained the potential energy that can compensate for the energy costs for generating defect pairs. Therefore the number of defect is determined by the balance between the gained potential energy and the energy of defect. Since the states of \( \theta_{\text{cr}} \) are only metastable there should exist the saddle points.

In order to know the director configurations when the system starts to transform we have to search for the saddle points in the energy surface \( \mathcal{E} \theta \) through which the director configuration can pass \( ^{210} \).

### 2.2 Nucleus for the spatial inhomogeneity

It is clear that the saddle points in the energy surface are given by the solution of

\[
\frac{\partial \mathcal{E} \theta}{\partial \theta} = K \frac{d^2 \theta}{dy^2} + \frac{1}{2} \mu_3 - \mu_2 \gamma
\]

\[
- \frac{1}{2} \mu_3 + \mu_2 \gamma \cos 2\theta = 0. \quad \text{5a}
\]

Multiplying \( \text{5a} \) with \( d \theta dy \) and integrating it we have

\[
K \int \frac{d \theta}{dy}^2 - 2 \mathbb{V} \theta = 2 U_0 \quad \text{6a}
\]

or

\[
K \int \frac{d \theta}{dy}^2 + \int \mu_3 - \mu_2 \theta
\]

\[
- \frac{3}{2} \mu_3 + \mu_2 \sin 2\theta = 2 U_0 \quad \text{6b}
\]

where \( U_0 \) is an integration constant.

To determine the value of \( U_0 \) we assume that the system is staying in a certain uniform state with \( \theta = \theta_u \) initially thus we have \( d \theta dy \mid y = 0 = 0 \) and \( \mathbb{V} \theta = \mathbb{V} \theta_u \). This results in \( U_0 = - \mathbb{V} \theta_u \). Then following Eq. \( 5 \) with \( U_0 = - \mathbb{V} \theta_u \) the excess energy of the critical nucleus from the uniform initial state \( \theta_u \) is given by

\[
\Delta E_{\text{Ncr}} = \Delta \mathcal{E} \theta_u = K \int \frac{d \theta}{dy}^2 dy. \quad \text{7}
\]

Firstly we discuss the case of \( \theta_u \neq \theta_u \neq \theta_u \). After introducing the deviation from the state \( \theta_u \) i.e. \( \Delta \theta = \theta - \theta_u \) and substituting it into Eq. \( 6 \) with \( U_0 = - \mathbb{V} \theta_u \) we obtain

\[
K \int \frac{d \Delta \theta}{dy}^2 = - \int \mu_3 - \mu_2 \Delta \theta
\]

\[
+ \frac{1}{2} \int \mu_3 + \mu_2 \cos 2\theta_u \sin 2\Delta \theta
\]

\[
+ \frac{1}{2} \mu_3 + \mu_2 \sin 2\theta_u \cos 2\Delta \theta - 1. \quad \text{8}
\]

The formal solution is

\[
\int d \Delta \theta \ - \mu_3 - \mu_2 \Delta \theta + \frac{1}{2} \mu_3 + \mu_2 \cos 2\theta_u \sin 2\Delta \theta
\]

\[
+ \frac{1}{2} \mu_3 + \mu_2 \sin 2\theta_u \cos 2\Delta \theta - 1 \int \Delta \theta = \pm \sqrt{\frac{\gamma}{K}}. \quad \text{9}
\]

Eq. \( 9 \) has been integrated numerically with the boundary condition of \( \Delta \theta = 0 = \Delta \theta_m \) \( \Delta \theta_m \) being the maximum deviation from \( \theta \). The results are shown in Fig. 3. We call this large amplitude nucleus \( \text{LAN} \).

In order to discuss the small amplitude nucleus \( \text{SAN} \) of the defect pair we expand the left side of Eq. \( 9 \) into powers of \( \Delta \theta \) and only keep the terms up to the order of \( \Delta \theta^2 \). We obtain when \( \mu_3 + \mu_2 \sin 2\theta_u > 0 \)

\[
\Delta \theta \mid y = \Delta \theta_{\text{m}} \ 1 + \sin \Omega_{\text{m}} y \quad \text{10}
\]

with
where $A = 0$, $B = 2 \sqrt{\mu_3 \mu_2}$ and $C = -\frac{2}{3} \mu_3 - \mu_2 \mu_3$. Then the solution of the above equation can be written as

$$\Delta \theta_{nc} = \Delta \theta_{nc}^* \frac{1}{\cosh^2 \frac{y}{2 \xi_c}} \quad 13$$

with

$$\Delta \theta_{nc} = -\frac{B}{C} = \frac{3}{2} \tan 2 \theta_s = \frac{3 \sqrt{\mu_3 \mu_2}}{\mu_3 - \mu_2} \quad 14$$

$$\xi_c = \sqrt{\frac{K}{2 \mu_3 \gamma}} \quad 15$$

in which we have set $\Delta \theta_{nc}^* y = 0 = \Delta \theta_m$. For the case of rod-like molecules $|\mu_3| \mu_3 | > 1 \theta_s \rightarrow \frac{\pi}{2}$ and $2 \theta_s \rightarrow \pi$ which reveals that $\Delta \theta_{nc}$ is very small.

Eq. 13 is a soliton-like solution which describes a pair of defects separated by a distance of $2 \xi_c$. Actually for the case where both $\mu_3$ and $\mu_2$ are negative and in the limit of $\mu_3 \approx \mu_2$ i.e. $\gamma = \mu_3 - \mu_2 \rightarrow 0$ Eq. 8 has a solution of sine-Gordon soliton \cite{20} of amplitude $\pi$.

$$\Delta \theta_{nc}^* y = 2 k \pi + 2 \arctan \left( \frac{0}{2 \xi_c} \right) \quad 16$$

with $\xi_c = \sqrt{\frac{K}{2 \mu_3 \gamma}}$.

2.3 Density of defects

By Eq. 11 that gives the periodicity of the spatial variation of the director the characteristic size $l$ of the director fluctuation is

$$l = \pi \frac{K}{\sqrt{\mu_3 + \mu_2 \sin 2 \theta_a}} \propto \gamma^{-\frac{1}{2}}$$

From the result of Eq. 15 the distance pair of defects which is called domain size in the literature of liquid crystals is

$$l = 2 \xi_c = \frac{2}{2 \sqrt{\mu_3 \mu_2}} \propto \gamma^{-\frac{1}{2}}$$

As we have only expanded the right side of Eq. 8 according to small $\Delta \theta_{nc}$ the above results are only suitable for the SANs of the defects. To find the distance between a pair of defects of LAN as shown in Fig. 3 we have to set $\Delta \theta = \Delta \theta_m + \phi$ and we obtain

$$\int \frac{d \phi}{d y} y^2 = \mu \Delta \theta_m + \phi^2$$

The above equation describes the exponential behavior.
of the pair of defects that have the solution of \( y = \pm \sqrt{\frac{K}{By}} \ln |\Delta \theta_m + \phi_p| \).

Fig. 3 shows that the top of the director configuration of critical nucleus pair of defects is very flat. To obtain the width of the flat top of the critical configuration we have to extend the above integration to an angle \( \phi_p \gg \Delta \theta_m \) but keep \( \phi_p \ll \pi \). This can be always true because \( \Delta \theta_m \) is small as shown by Eq. 14. The flat top of the nucleus pair of defects therefore has an extension \( 2y_p \) with \( y_p \) given by

\[
y_p = \pm \sqrt{\frac{K}{By}} |\Delta \theta_m + \phi_p| \approx \pm \sqrt{\frac{K}{By}} \ln |\Delta \theta_m|
\]

as \( \phi_p \) is large and makes almost no contribution to \( y_p \). This again tells us that the distance between a pair of defects domain size is proportional to \( \gamma^{-1/2} \).

The density of defects \( \rho \) can be simply estimated. We consider a system of length \( L \) along which there are \( m \) pairs of defects with amplitude of \( \pi \). According to Fig. 8 the directors between two pairs of defects are staying in one of the minimum of \( \theta_1 \) say \( \theta_G \) while the directors in the flat top of the defect pair are located in the minimum next to \( \theta_G \) i.e. \( \theta_G + 1\pi \) which loses potential energy \( |y_p| \mu_3 - \mu_2 \pi \). The flat top does not contribute to the excess energy of the defects \( \Delta E_n \). According to the energy balance we finally obtain

\[
\rho = \frac{m}{L} \propto \gamma^{-1/2}.
\]

This simple scaling relation has been confirmed experimentally.

However the domain size should not be smaller than the molecular or interaction characteristic length \( l_c \) therefore there is a transition from the defect production and shear-induced homogenization at the critical shear rate

\[
\dot{\gamma}_c = \frac{2K}{\mu_3 \mu_2 l_c^2}
\]

which is called the upper boundary of Region II viscosity in the literature.

2.4 Energy barrier for production of defects

For the critical nucleus the energy barrier across the saddle is \( \Delta E_{nc} \). In the limit of small amplitude nucleus which is defined by Eq. 13 \( \Delta E_{nc} \) can be calculated analytically

\[
\Delta E_{nc} = \frac{8}{15} \frac{K \Delta \theta_{nc}^2}{\sqrt{2 \gamma}} \frac{K}{\mu_3 \mu_2 \gamma}
\]

\[
= \frac{24 \mu_3 \mu_2}{\gamma} \sqrt{2K \gamma} \sqrt{\mu_3 \mu_2}.
\]

For the case of periodic nucleus the energy barrier for one pair of defects is

\[
\Delta E_{np} = \frac{\pi}{8} \mu_3 \mu_2 \sin \theta_a < 0 \quad \mu_3 - \mu_2 \sin 2 \theta_a > 0 \quad \mu_3 + \mu_2 \cos 2 \theta_a > 0 \quad \mu_3 - \mu_2 \cos 2 \theta_a > 0
\]

\[
\cdot \sqrt{K \gamma} \mu_3 + \mu_2 \sin \theta_a.
\]

It is seen that energies of the states \( \Delta \theta_{nc} \) and \( \Delta \theta_{np} \) \( \Delta E_{nc} \) and \( \Delta E_{np} \) are stationary with respect to small changes in the director configuration.

We must note that \( \Delta E_{np} \) becomes very small when \( \mu_3 + \mu_2 \cos 2 \theta_a > 0 \quad \mu_3 - \mu_2 \sin 2 \theta_a > 0 \) and \( \mu_3 - \mu_2 \cos 2 \theta_a > 0 \) when both \( \mu_2 \) and \( \mu_3 \) are negative and near to \( \theta_a \). This means that the system will overcome the barrier \( \Delta E_{np} \) easily and the periodic director patterns emerge when the system is occasionally passing through the unstable stationary state \( \theta_a \).

Many experimental observations indicate that when the shear strain is as low as about \( 1 \sim 10 \) units the director is rotating around the vorticity axis in the shear plane the periodic bands emerge with the band axis perpendicular to the flow direction i.e. parallel to the vorticity axis. Then it transforms to worm-like or stripe texture. The optical measurement has shown that in the worm-like texture the director of the molecules is in the flow direction and has significant degree of orientation.

It should be pointed out that in Fig. 4 the angles of \( \theta_s \) and \( \theta_a \) are reduced artificially for the clarity of the figure. In reality \( \theta_s \) and \( \theta_a \) are very close to \( \theta \) 2 and \( \theta \) 2 respectively. It is important to note that in the second and fourth quadrants \( \mu_3 + \mu_2 \sin 2 \theta_a < 0 \) while it is negative in the first and third quadrants when \( \mu_3 \) and \( \mu_2 \) are negative.

As \( \theta_a \) is in the first quadrant where \( \mu_3 + \mu_2 \sin 2 \theta_a < 0 \) the fluctuation will lead the system to pass through the saddle and the pairs of defects described by Eq. 13 will be nucleated. However

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Because $\theta_\ast$ is very close to 0°, the fluctuation can occasionally lead the system to pass through the potential barrier $\Delta V$ described by Eq. 4 especially when the shear rate is low and thus $\Delta V$ is very low too. The director can either overcome the barrier to transform to the next minimum of $\theta_\ast$ or on the way of passing through the potential hill the fluctuation will lead the system to leave the potential hill and nucleate the periodic structures described by Eq. 13 due to $\mu_3 + \mu_2 \sin 2\theta_\ast > 0$ in the second quadrant. We should note in advance that the periodic solution is unstable therefore it can only be observed as transient pattern.

Of course the system will select energetically in favorable path. We should point out that $\Delta E_{ep}$ and $\Delta E_{nc}$ are proportional to $\gamma^{\Omega 2}$ while $\Delta V$ is proportional to $\gamma$. Therefore there should exist a critical shear rate in the form

$$\gamma_c = \frac{24 \mu_3 \mu_2 \Omega^2}{2 \pi \mu_3 - \mu_2 \Omega L^2} \pm \mu_3 - \mu_2 \frac{\pi}{2} \arctan \left( \frac{\mu_2}{\mu_3} \right)$$

with $L$ being the length of the system. In the above equation the upper sign is for the case of negative $\mu_2$ and $\mu_3$ and the lower sign for the positive $\mu_2$ and $\mu_3$.

Eq. 17 tells us that when the shear rate is lower than the critical $\gamma_c$ the director prefers to overcome the potential barrier $\Delta V$. As we have just discussed the periodic pattern bands will be easily nucleated in this case. However when the shear rate is higher than the critical value the only possibility is to nucleate the critical pairs of defects. In addition the periodic pattern emerges from the state around the unstable stationary state $\theta_\ast$. The system will find some lower paths and eventually transform to the next minimum of the potential energy as depicted in Fig. 2 and then the critical pairs of defects can be nucleated. We believe that this is responsible for the experimental fact that the bands parallel to the vorticity axis can be observed only at lower shear rate and lower shear strain units and the defects or called worm-like textures in higher shear strain units. On the other hand if the shear rate is higher than the thermal fluctuation i.e. $\Delta E_{nc} \sim \gamma^{\Omega 2} \gg kT$ then the nucleus of the defects cannot be generated except we have some other noise sources such as mechanical noise. In fact during shear flow the mechanical noise is inevitable due to the small roughness of the shear plates or mechanical vibrations. This argument is consistent with the experimental observation that the critical shear rate for the defect formation is strongly reduced by introducing large amplitude mechanical noise. We believe that the mechanical noise provides some fluctuations of the director field and makes the system’s method overcome the energy barrier for nucleation of defects.

### 3 The stability of the pattern

According to Eq. 5 the motion equation for $\Delta \theta$ is written as

$$\gamma_1 \frac{\partial \Delta \theta}{\partial t} = K \frac{\partial^2 \Delta \theta}{\partial y^2} + \frac{1}{2} \gamma \mu_3 - \frac{\pi}{2} \mu_2 \Omega L^2 \pm \mu_3 - \frac{\pi}{2} \mu_2 \gamma \arctan \left( \frac{\mu_2}{\mu_3} \right)$$

The stationary solution for the above equation has been obtained in last section. Now we assume another deviation from $\Delta \theta$ $y_0$ by an angle of $\partial \theta$ $y_0$ and therefore $\Delta \theta$ $y_0'' = \Delta \theta$ $y_0$ $+ \partial \theta$ $y_0''$. Expanding it to the first order of $\partial \theta$ $y_0'''$ we obtain the motion equation for $\partial \theta$ $y_0'''$

$$\gamma_1 \frac{\partial \Delta \theta}{\partial t} = K \frac{\partial^2 \Delta \theta}{\partial y^2} + \mu_3 + \mu_2 \gamma \cos 2\theta_\ast \sin 2\Delta \theta + \sin 2\theta_\ast \cos 2\Delta \theta \partial \theta.$$
By retaining the first order of $\Delta \theta\ dy$ we have

$$\gamma_1 \frac{\partial \theta}{\partial t} = K \frac{\partial^2 \theta}{\partial y^2} + \mu_3 + \mu_2 \dot{y}$$

$$+ 2 \cos 2 \theta_0 \Delta \theta_a + \sin 2 \theta_a \partial \theta \ . \ \Box \ 18\Box$$

As $\theta_a$ and $\Delta \theta\ dy$ are independent of time the solution of the above equation can be assumed to be in form

$$\dot{\theta} \ y(t) = \dot{\theta} \ y[exp] = \lambda t \ . \ \Box \ 19\Box$$

Substituting Eq. 19 into Eq. 18 we have the eigen-value problem of

$$L \dot{\theta} \ y = - \lambda \gamma_1 \dot{\theta} \ y \ . \ \Box \ 20\Box$$

The operator is defined as

$$L = K \frac{\partial^2}{\partial y^2} + \Box \ \theta_a \Box \Delta \theta_a \Box$$

with

$$\Box \ \theta_a \Box \Delta \theta_a \Box = \mu_3 + \mu_2 \dot{y} \ \Box \ \Delta \theta_a + \sin 2 \theta_a \Box$$

In the case of critical nucleus the eigen-value equation is written as

$$\frac{\partial^2 \theta}{\partial y^2} + \left( \frac{\lambda \gamma_1}{K} - \frac{1}{\xi_c^2} \right) + \frac{3}{\xi_c^2 \cos \theta \ \sqrt{\frac{\gamma}{2 \xi_c}}} \ \Box \ 21\Box$$

where $\xi_c$ is defined in Eq. 15. Eq. 21 is similar to the the equation for describing single particle moving in a potential defined by Eq. 13. The above eigenvalue equation is similar to the driven and overdamped sine-Gordon equation21. The eigenvalue problem of the above equation can be solved using Landau and Lifshitz’s method20. We have found the eigenvalues for the localized modes

$$\lambda_n = \frac{K}{\gamma_1 \xi_c} \left[ 1 - \frac{3}{4} \frac{n^2}{\xi_c^2} \right] \ 0 \leq n \leq 3 \ .$$

The corresponding eigen-functions are

$$\dot{\theta}_{0c} = C_0 \ \xi_c \ \text{sech}\left[ \frac{\gamma}{2 \xi_c} \right]$$

$$\dot{\theta}_{1c} = C_2 \ \xi_c \ \frac{\sinh \left[ \frac{\gamma}{2 \xi_c} \right]}{\cosh \left[ \frac{\gamma}{2 \xi_c} \right]}$$

$$\dot{\theta}_{2c} = C_1 \ \xi_c \ \frac{1 - 4 \sinh \left[ \frac{\gamma}{2 \xi_c} \right]}{\cosh \left[ \frac{\gamma}{2 \xi_c} \right]}$$

where $C_0$ and $C_2$ are normalization constants $\xi_c$ is defined by Eq. 15. The unstable mode $\dot{\theta}_{0c} \ y$ with eigenvalue $\lambda_{0c}$ describes the contraction or extension of the pair of defects. The second eigenmode $\dot{\theta}_{1c} \ y$ with eigenvalue $\lambda_{1c}$ describes the translation of the defect pair. The third eigenmode $\dot{\theta}_{2c} \ y$ with eigenvalue $\lambda_{2c}$ describes the expansion or contraction of the width of each defect. It is seen that the energy decreases in the direction of the unstable localized eigen-mode $\dot{\theta}_{0c} \ y$ and increases in the stable localized eigen-mode $\dot{\theta}_{2c} \ y$. Following the discussion of Buttiker et al.21 the curvature near the saddle of the energy surface in the direction of certain mode $n$ is proportional to $\lambda_n$. Therefore the saddle of the energy surface is flat in the direction of $\dot{\theta}_{2c} \ y$ and is very flat in the direction of $\dot{\theta}_{1c} \ y$. This also implies that the production of defects during shear flow can easily happen.

4 Stability and the traveling velocity of the soliton

Due to the existence of macroscopic shear flow, the drift of the pair of defects will be essentially in the flow direction. To investigate the propagation of these driven defects we search for the stationary traveling waves $\Box \ z \Box$ which depend on $y$ and $t$ only in the combination $z = y + ut$ where $u$ is the propagation velocity of the defect pair in the minus $y$ direction. In a frame for a stationary traveling of the defect pair with velocity $u$ Eq. 1 becomes

$$K \frac{\partial^2 \theta}{\partial z^2} - \mu_1 \frac{\partial \theta}{\partial z} + \frac{4}{3} \mu_3 - \mu_2 \dot{y}$$

$$- \frac{4}{3} \mu_3 + \mu_2 \dot{y} \ \cos \theta = 0 \ . \ \Box \ 22\Box$$

By linearizing Eq. 22 with respect to a small perturbation $\dot{\theta} \ y \Box$ to soliton $\Delta \theta \ y \Box$ of Eq. 16 the motion equation for $\dot{\theta} \ y \Box$ is written as

$$K \frac{\partial^2 \theta}{\partial z^2} - \mu_1 \frac{\partial \theta}{\partial z} + \Box \ \mu_3 + \mu_2 \dot{y} \ \sin 2 \theta_s \cdot \ \Box \ \dot{\theta} = 0 \ . \ \Box \ 23\Box$$

Actually for the sine-Gordon soliton described by Eq. 16 it is well known that the traveling of the soliton is stable against the small perturbation21.27.

We have numerically analyzed the flow of $\frac{d \theta}{d z} \ \Box$ for Eq. 22 and the result is shown in Fig. 5. It is found that there are two types of solutions. The first solitary solution emerges from $\Box 0 \ \Box$ spiraling to $\Box 0 \ \Box$ which is unstable against small perturbations. This solution corresponds to our solution of periodic nucleus Eq. 10. The second solitary solution departs from a stable uniform state $\theta_{0c}$ and approaches the next neighboring state $\theta_{2c+1}$. This solution is stable against small perturbations. The flow of $\frac{d \theta}{d z} \ \Box$ reveals that the critical nucleus generated from the stable state $\theta_{2c}$ is stable.
while the periodic nucleus generated from unstable state $\theta_{d=0}$ is unstable. If the system accidentally goes to the unstable state $\theta_{d=0}$ due to some mechanical or other noises the traveling wave will be spiraling away from that state and get into the stable solution. This character of the flow diagram is coincident with the qualitative discussion given in Sec. 2. It agrees with the analysis given by Buttiker et al.\cite{29} for the over-damped sine-Gordon soliton.

Fortunately the travelling velocity of defects $u$ can be calculated analytically. Following Ref. 21\cite{24} we obtain

$$u = \frac{\pi}{4} \sqrt{\frac{K \gamma}{|\mu_3 + \mu_2|}}$$

when both $\mu_3$ and $\mu_2$ are negative. The velocity of the stationary traveling soliton $u$ can also be determined by a numerical method introduced by Buttiker et al. The values of $u$ obtained by numerically solving Eq. 22\cite{24} are shown in Fig. 6 and compared to the analytical results\cite{24}.

Fig. 6. The shear rate dependence of the propagation velocity of a pair of defects. In the calculation\cite{24} $\mu_2$ and $\mu_3$ have been set at $-0.4$ and $-0.04$ which are corresponding to the value of 5CB. The dots are obtained by numerical simulation of Eq. 22\cite{24} and the solid line is calculated from Eq. 24\cite{24}. It follows the relation of $u \propto \sqrt{\gamma}$.

The theory has proved that the distance between a pair of defect or the periodicity of the band pattern namely the characteristic size of domains\cite{24} follows the relation of $l \propto \gamma^{-a}$ with $a = 2/3$. Compared to the experimental results of Mather et al.\cite{24} however the experimental $a$ value for 5CB is 0.63. The deviation may come from the following reasons. First\cite{24} the experiment was done under the torsional flow field. Second\cite{24} since the production of defects is the intrinsic behavior of the flow-aligning nematics it makes the connection between flow-aligning and -tumbling unclear. Therefore\cite{24} in many experiments one is not sure whether the domain size measured in experiment is generated by director tumbling of a flow-tumbling nematics or by defect production of flow-aligning nematics. This may introduce some uncertainties into the comparison between theory and experiment. Actually\cite{24} in Ref. 16\cite{24} the measured domain size could be the width of strips formed from the flow-tumbling nematics which does not belong to the category discussed in this paper. Thirdly\cite{24} the back-flow effect neglected here may also alter the exponent value $a$. The director may have the component out of the shearing-plane which may also modify the value of $a$. Finally\cite{24} in the theoretical analysis\cite{24}.

5 Summary and conclusions

In this paper it is found that there are two types of spatial patterns can be nucleated unstable periodic nucleus and stable critical nucleus. The periodic pattern could be observed at low shear rate and low shear strain value. However the periodic pattern can only be observed as a transient pattern as it is unstable against small disturbances. When the shear rate is higher than a critical shear the spatial pattern can only be formed through the critical nucleation of soliton-like structure i.e. pairs of defects.
we have assumed that the director is uniform in $x$-direction. However it is also plausible to have the spatial structures in that dimension. Certainly on this aspect it deserves careful experimental and more sophisticated theoretical analysis.

We have noted that the mechanical noise introduced during shear is crucial for the system to overcome the barrier for the production of defects. It interprets the experimental results of Mather et al.\cite{Mather}. It can be expected that the mechanical noise will be enhanced when shear rate is high due to the inevitable non-uniform thickness of the cell or the roughness of the plates.

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References


