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The Transition to Turbulence in Nematic Liquid Crystals†

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The article is divided in two parts.

In part I we review the present state of knowledge on the problem of the transition to turbulence in isotropic liquids and we discuss analogies/differences with the case of nematics. In the well known Rayleigh-Bénard case, experiments on ordinary liquids show that one must distinguish between confined and extended geometries (small or large "aspect ratios"). This difference is quite general and arises from the more or less large number of variables required to describe the structure. In confined geometry a Ruelle-Takens type of sequence seems relevant, with subharmonic bifurcation or intermittency as special cases. In extended geometry, slowly evolving imperfect structures (which may arise from an instability of the phase of rolls) result in a broad noise which can be viewed as a precursor of turbulence.

In nematic liquid crystals (NLC) much less is known on the transition to turbulence. Nematic flows are very strongly non-linear and are in large part controlled by the director field distortions. We review briefly the transition to turbulence in electrohydrodynamic (EHD) instabilities. It is shown to roughly follow the same type of scheme as ordinary Rayleigh-Bénard convection but mechanisms involved have not yet been unambiguously isolated. The particular role of the director field dynamics is more clearly seen in the case of flow instabilities. We recall the principal situations of interest, namely

- i) when the viscous torque coefficient α_3 is positive and the director lies in the plane of velocity and velocity gradient so that "tumbling" can occur and
- ii) when the nematic in homeotropic geometry is submitted to an elliptical shear: the transition to turbulence then occurs through a gradual loss of spatial coherence analogous to some steps observed in the EHD case.

The bibliography though already extended is far from complete. It is mainly experimental but may serve as a useful starting point for a reader who would be interested by a theoretical approach of the transition to turbulence in NLC.

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In part II we study more thoroughly the "tumbling" phenomenon and conjecture the statistical properties of a turbulent state which would bifurcate quasi directly from the laminar state in a nematic with $\alpha_1 > 0$ and aligned in the direction of the Poiseuille flow. A numerical simulation allows to determine the "tumbling" threshold with as few simplifying assumptions as possible and starting with Ericksen-Leslie equations. We show that the tumbling instability is first order-like and we give indications on its dynamics. Motion of defects that can nucleate from the "tumbled state" is studied qualitatively. This leads directly to some predictions for the kind of turbulence observed by Gähwiller in his experiment on HBAB.

PART I: GENERAL REVIEW

I INTRODUCTION: THE TRANSITION TO TURBULENCE IN ISOTROPIC LIQUIDS

The problem of the transition to turbulence in dissipative systems has received a reviewed interest since the publication of the paper by Ruelle and Takens. It came and profoundly revised the classical Landau-Hopf scheme of an infinite series of bifurcations leading to chaos through quasi-periodicity at the limit of infinite stresses. This and other abstract mathematical approaches, complemented and stimulated by numerical experiments on explicit models have put the stress on possibly "strange" properties of non-linear systems which can be deterministic in the short term but quite unpredictable in the long term; hence a new insight "on the nature of turbulence". Experimental evidence of the overall correctness of this picture is very recent. It has been gained mainly in studying Rayleigh-Bénard (RB) convection and Taylor instabilities in usual isotropic liquids. The spirit of this novel approach is rapidly expanding in other fields such as chemical instabilities but experiments in nematics conducted along these lines are still very scarce.

In fact, experiments suggest that there are several ways to turbulence. Reproducibility is not always the rule but parameters which control these different ways begin to be recognized; these are essentially:

Physical parameters of the fluid such as the Prandtl number Pr in RB convection, which control the physical nature of the secondary instabilities: at low Pr oscillations seem related to Busse's mechanism ^{13,7a} while at high Pr instabilities of the thermal boundary layer play the dominant role. ^{9a}

Geometrical parameters, which decide from the spatial structure of unstable modes and, to a certain extend, control the form and the intensity of the coupling between these modes. In general the instability mechanism is associated with a particular direction (the gravity direction in case of buoyancy driven convection) and the instability threshold is usually related to the dimension d of the experimental set up in that direction, which in addition fixes the dimension of the domains, roll, cell, . . . which appear above the threshold. Roughly speaking the "aspect ratios" (the ratios between other dimension)

sions of the apparatus and that dimension d) give the number of cells which will set in, and more or less, the number of degrees of freedom of the system which can be easily excited in the non-linear regime above the threshold.

In addition, the history of the experiment may play a role. According to the way the external forcing stress has been switched, the system may "choose" one or another of the spatial configurations which are nearly equally possible close to the instability threshold. This may be important not only in the large aspect ratio limit (large number of cells — many possible configurations) but even in the small aspect ratio limit where the system may "choose" between a small number of possible spatial structures.

In confined geometry (small aspect ratios) a small number of degrees of freedom can be excited and a picture "à la Ruelle-Takens" (R-T) is expected to hold. In this picture, turbulence is understood mostly as "temporal chaos," the apparent "spatial chaos" resulting from the chaotic evolution of the amplitude of a small number of well defined spatial modes as in the Lorenz model.³

The R-T general scheme is: time independent regime \rightarrow periodic regime (Hopf bifurcation) \rightarrow biperiodic regime (Hopf bifurcation) \rightarrow chaos. Possibility of a triperiodic regime is left open but chaos should appear at finite distance of the first instability threshold after asmall number of bifurcations.

This is to be contrasted with the Landau-Hopf (L-H) scheme which involves an infinite series of Hopf bifurcations each adding a new incommensurate frequency, chaos being obtained through quasi-periodicity in the limit of infinite stresses.

Up to now only special cases of this R-T scheme have been successfully interpreted among experimental results. These are mainly

—an infinite cascade of bifurcations^{7b} which occurs in case of strong resonance between the first and second frequency. Bifurcation thresholds have an accumulation point at finite stress and the entire sequence should be counted for one; this is very different from L-H scheme which assumes incommensurate frequencies. Note that chaos can appear after only few successive subharmonic bifurcations for still obscure reasons.^{6a}

—a "continuous" transition to chaos with an "intermittent" destabilization of either a periodic state^{9d} or a quasi-periodic state; "intermittency" means here a random alternation of regular "laminar" phases and irregular "turbulent" bursts; "continuous" means that when the stress is increased the proportion of time spent in laminar phases steadily decreases.

These two particular sequences seem well understood from a theoretical point of view even if one cannot prove rigorously the explanations in deriving explicit models. These explanations rest on simplified discrete models of the form

$$x_{n+1} = f(x_n),$$

the subharmonic case¹⁵ corresponding to $f(x_n) = ax_n(1 - x_n)$ and the intermittent destabilization of a periodic state^{16a} to $f(x_n) = x_n + x_n^2 + a$ (+ a periodic condition on x).

Theory for other experimentally observed sequences such as the growth of low frequency broad band noise is presently an active research field. 17

The relevance of the R-T bifurcation theory is not so obvious in the case of extended geometry: large aspect ratios and large number of degrees of freedom excited quite close to the first instability threshold. In fact, R-B convection experiments in low Prandtl number fluids^{7a,8} have shown that noise appears at unexpectedly low stresses well before coherent time oscillations are expected to take place. Evidence is growing for a certain kind of spatiotemporal chaos resulting from a permanent evolution of the structure; the many degrees of freedom interfering to give unstable phase fluctuations^{16b} or defects^{9a} in the convective structure. Such a behavior has been observed also in high Prandtl number fluids¹⁸ and even in the case of Taylor instability. ^{10c} This spatio-temporal chaos is not well understood but should perhaps be related to the criticism of the Ruelle-Takens scheme developed by Monin¹⁹ for whom true turbulence must involve an erratic motion on several spatial scales, which will be the case if random creation-annihilation of more or less local defects occurs in the statistically permanent regime.

Before this recent effort to relate turbulence to mathematical properties of non-linear systems, theory was mostly devoted to the identification of unstable modes in the non-linear regime^{20,21} and experiments were conducted either to verify these predictions^{22,23} or to set up a phenomenology of the transitions to turbulence.²⁴ As we shall see below, only this last aspect is represented in present literature on instabilities in nematics since with very few exceptions, non-linear theory above threshold has not yet been developed.

II SPECIFICITIES OF NEMATICS

In order to better situate the case of nematics let us point out possible a priori differences: they are all linked to the presence of the additional director field.

First, nematics are much more strongly non-linear than isotropic liquids which are systems of the "hydrodynamic type" in the sense of Obukov²⁵ i.e. with a quadratic coupling between modes originating basically from the so called "convective term" $V.\nabla(...)$. Here dominant non-linearities come from the fact that the director field can be easily distorted. Even though Frank elasticity and Leslie viscosity are locally linear phenomena (i.e. in a frame linked to the local director) macroscopic equations in the laboratory frame result from a strongly non-linear change of coordinates as soon as deviations from uniform alignment are no longer infinitesimal. "Tumbling" to be studied in Part II is an example of non-trivial behavior one can expect.

In the case of chemical instabilities, ¹¹ equations are neither of the "hydrodynamic type" but up to now not very novel features have been brought in the field of transitions to turbulence when compared to classical hydrodynamic instabilities except perhaps for specific spatial phenomena such as the instability of a reaction front due to "phase turbulence". ²⁶

Second, one can expect that the anisotropy of nematics be an important characteristic since in most cases the structure and orientation of the convective structure are controlled by the unperturbed director field. Thus orientational boundary conditions will play an important role. Homeotropic or conical anchoring will leave us with a situation analogous to isotropic Rayleigh-Bénard convection: i.e. a rotational invariance (at least locally) in planes parallel to the boundary. On the contrary, planar or oblique anchoring will break this invariance. In certain cases a bulk phenomenon linked to the nematic anisotropy can also lead to a well defined weakly degenerated pattern in much the same way as the direction of flow does in Taylor instability. Thus in general, degeneracy will be strongly reduced in nematics when compared to isotropic liquid convection.

Finally, in addition to defects in the convective structure such as dislocations in the otherwise regular two dimensional roll pattern, with nematics we add the possibility of topological defects of the director field itself. As will be sketchily discussed in Part II, turbulence can arise in nematics by nucleation-annihilation of such defects. This occurrence is not special to nematics but can be found also in other ordered media such as superfluid Helium where turbulence is understood as a dense random network of vortices of normal Helium in a matrix of superfluid Helium.

In the following we shall review some selected experimental situations where transition to turbulence have been reported:

Electrohydrodynamic instabilities Rayleigh-Bénard instabilities Certain flow experiments.

The basic mechanisms which drive these instabilities are generally sufficiently understood (see the review articles: Refs. 27-34) but nearly nothing is known theoretically on the stability of non-linear solutions above the instability thresholds nor on the dynamics of orientation defects in the strongly distorted regime.

III THE TRANSITION TO TURBULENCE IN ELECTROHYDRODYNAMIC INSTABILITIES

This problem is very well known since "dynamic scattering" was the first turbulent-like property of nematics which received applications. However it is not very well understood. The review we shall give of this topic may appear of "zoological" interest only but in our opinion, no convincing general scheme exists to classify experimental facts. So we have preferred to give a selected (and perhaps partial) bibliography accompanied by some critical comments. These should be understood as a starting point for further studies.

Several mechanisms have been recognized to be relevant;³² mainly

The Felici mechanism of charge injection³⁵

The Carr-Helfrich mechanism which combines charge focalization and dielectric anisotropy effects. 36,37

Anomalous charge focalization in tilted geometries³⁸ Flexoelectric effects.³⁹

The experimental situation is then difficult to clarify since the respective weight of these mechanisms has to be evaluated in each specific case. Moreover to the usual problems raised by electrical phenomena in dielectric liquids one can add more or less uncontrollable secondary effects linked to the properties of molecular anchoring under electrical field. However the technical ease for controlling the stress may prove valuable if one succeeds in choosing a well defined experimental situation and takes care of analyzing the sources of parasitic effects.

Here we shall restrict ourselves to the case of the "conduction" (low frequency) regime with planar anchoring in a sandwich geometry with the electrical field E perpendicular to the cell. When charge injection effects can be eliminated and the cell is not too thin, the Carr-Helfrich mechanism is expected to account for the first instability. Transition to turbulence in that case has been studied more especially by Hirakawa and coworkers and by Ribotta at Orsay. Other situations arise at high frequencies ("dielectric" regime) or with oblique or homeotropic alignment or in very thin cells. Mechanisms involved in these cases seem not so clearly isolated. Finally apart from this sandwich geometry with $E \perp$ to the cell we note that the opposite case, $E \parallel$ to the cell, has also been studied extensively. Experiment performed up to now did not concentrate on the problem of the transition to turbulence but rather on the strongly turbulent case.

1 Qualitative aspects of the transition to turbulence for Williams Domains.

Above the Williams Domains threshold $W_{\rm WD}$, the wavelength of the roll is observed to decrease steadily and oscillations have been reported by many groups; 27,40,47,48 the frequency of these oscillations seems to increase linearly with the distance to $V_{\rm WD}$. 27,47 This regime has been called Fluctuating Williams Domains (FWD) by Hirakawa and coworkers. It is not yet completely clear whether or not truely stationary rolls can be observed in a range of Voltage values immediately above $V_{\rm WD}$, i.e. if $V_{\rm FWD}^2$ is strictly larger than $V_{\rm WD}$.

At a second threshold a more or less rectangular grid pattern (GP) appears.

Then the grid begins to move giving the fluctuating grid pattern (FGP) or Quasi-GP.⁴⁰

Finally turbulence sets in, first under the form of a spatial chaos at roughly the scale of GP and with the creation of some disclination loops (Dynamics Scattering DSMI) and then under the form of fluctuations at a much smaller scale (DSM2) nucleated rather locally but then rapidly invading the whole nematic film.⁴⁹

2 Discussion

Current interpretations involve the comparison with the RB instability case as studied by Busse and Whitehead or Krishnamuti. A detailed comparison is not so obvious; indeed, physical mechanisms are very different. For example in RB Convection, the wavelength of the rolls increases above the threshold, this while the opposite behavior is observed above the voltage threshold $V_{\rm wD}^{\rm c}$. In both cases there is not yet any clear explanation. Lateral boundaries are suspected to play a role for wavelength selection in the RB case. For nematics either a condition of maximum linear growth rate or maximum distortion have been invoked but these are simply assumptions which are known to have counter-examples. In fact a comprehensive non-linear theory which does not assume a definite wavelength from the start, has not yet been worked out; only one dimensional solutions exist which do not allow for wavelength adjustment.

The origin of oscillations is also very mysterious. Stability analysis of present non-linear solutions would be meaningless due to their schematic character. It has been suggested⁴⁷ that they could be related to Busse's mechanism of vertical vorticity generation. ^{13a} This was appealing, however Busse's theory is expected to work at low Prandtl number i.e. when vorticity fluctuations relax much more slowly than temperature fluctuations. Here vorticity is the most rapidly fluctuating quantity and velocity fluctuations are more or less slaved to orientation and charge fluctuations so that one expects oscillations to derive from a non-linear coupling between these two last quantities. (Moreover in Busse's theory the frequency varies as the amplitude of convection which grows as the square root of the distance to the threshold and not linearly with it as it seems to be the case for WD).

Mechanisms which result in striations perpendicular to the WD have been suspected to enter play for GP like structures.⁵⁸ In fact the situation as described by Ribotta⁴¹ leads to think that GP is a time independent regime tightly linked to the oscillations which occur at Voltages slightly lower or slightly larger so that the existence of true bifurcation points is even questionable. Oscillations at lower voltages involve pieces of rolls which periodically rotate more and more up to a point where the system is locked on a time independent rectangular pattern. At higher voltages oscillations start again and one can

observe a regular alternation of more or less aligned broken rolls with a rectangular pattern (exchange of dimension). Moreover chaos seems to grow rather continuously by loss of spatial coherence. This description of facts seems in good general agreement with that presented by Hirakawa et al. for the WD case, which implies that their experimental conditions are rather similar.

To conclude this section, let us stress that apart from the basic mechanism of the first instability which has been checked with sufficient accuracy, 59 nearly nothing is known on the transition to turbulence in Electrohydrodynamic instabilities from the theoretical view point.

IV THERMAL INSTABILITIES

Modifications involved by heat focalization in nematics when compared to isotropic liquids are now well understood. They can lead to rather exotic situations since in a homeotropic slab, time independent convection occur when heated from above while oscillatory convection can set in when heated from below. 62,63

Up to now except the experimental work by T. Riste et al., ¹² to our knowledge nothing has been devoted to the transition to turbulence in Rayleigh-Bénard convection of nematics. No theoretical account of this last work has been given so far. The experiments correspond to a case of confined geometry with a priori few modes involved. Indeed a sequence with time-independent, time periodic and chaotic convection has been observed. ¹² To a large extent the problem of orientational boundary conditions has been eliminated since a magnetic field was used to orient the nematic. It is not clear whether and how this can simplify the analysis.

Other experiments²⁷ were rather devoted to the vicinity of the linear instability threshold as determined by usual normal mode analysis.⁶⁴⁻⁶⁶ Non-linear approaches are at their very beginning and make use of simplifying assumptions such as "free-free" boundary conditions for the velocity fluctuations.⁶⁷

A comparison between Williams Domains and RB convection in planar geometry would certainly help to clarify the mechanisms involved in the EHD cascade of instabilities.

In homeotropic geometry slightly above the threshold for roll convection one observes a square pattern⁶¹ yet unexplained. From a formal point of view, restored rotational invariance in the plane of the fluid layer could have led to an interesting comparison with usual RB convection in extended geometry.

V FLOW INSTABILITIES

Flow instabilities have a two fold interest:

—first they involve the coupling between orientation and velocity in a cru-

cial way, which leads to hydrodynamic instabilities with no equivalent in isotropic liquids and

- —second they may come into play as secondary instabilities in the case of primary instabilities generated by more standard mechanisms. Here we shall quote some of the results obtained up to now and classify them under two headings:
 - -experiments of the viscometric type,
 - -experiments of a special type.

1 Experiments of the viscometry type

As is well known, the 3 Miesovicz geometries give a first framework for further classification; and the sign of the coefficient α_3 (viscous torque coefficient) gives another one.

The case where the director is perpendicular to both the velocity and the velocity gradient was not much considered at the beginning since this orientation is basically unstable²⁹ (when $\alpha_3 < 0$). But in fact this geometry has given a rich family of instabilities^{68,69} which allowed for a detailed comparison between experiment and theory as far as the instability thresholds⁷⁰ and the first non-linear stage are concerned.⁷¹ Not much is known about the next steps to turbulence.

When the director lies in the plane defined by the velocity and the velocity gradient, the situation seems much more specific of nematics since viscous torques play a role not at first order in fluctuations as before but at order zero. In strong shear the nematic orients itself⁷² in the flow at the Leslie angle θ_L which exists as long as α_2 and α_3 have the same sign i.e. both negative since α_2 is expected to be negative for rod shaped molecules. When $\alpha_3 > 0$ the Leslie angle no longer exists. A well defined orientation can exist in the limit of low shears as long as elastic torques can compensate the two viscous torque contributions which can no longer balance each other. Normal mode stability analysis was developed by Pikin. First evidence of a nematic with $\alpha_3 > 0$ came with Gähwiller's experiment followed, a review of which can be found in part II where we develop the idea that Poiseuille flow in a nematic with $\alpha_3 > 0$ and a director parallel to the plane of velocities could supply a unique opportunity to observe a kind of turbulence rather special to nematics.

2 Other experiments

As far as we know, another situation has lead to the observation of a complete sequence of transitions from laminar to turbulent state in nematics: the elliptical shear flow with homeotropic anchoring. In the unperturbed basic flow the director rotates uniformly on a cone. Then a system of parallel rolls appear above a certain threshold, 75,76 the orientation of the rolls being controlled in the bulk by the ellipticity of the shear.

The corresponding mechanism is rather well understood. ⁷⁶ The structure of rolls is very regular but one can study quite carefully the natural birth or death of a pair of dislocations, ⁷⁷ which may be of a great interest on more general grounds. After the rolls come squares ^{78–80} (or rather lozenges) and sometimes hexagons (Note that squares can also appear as 1st instability when symmetry is restored: i.e. in case of circular shear). Then turbulence enters as a gradual loss of spatial coherence with well "crystallized" regions separated by grain boundaries. The size and total area of the "crystallites" decrease as the shear increases and a situation analogous to "dynamic scattering" prevails at end. A tentative interpretation has been given in terms of two-dimensional melting. ^{78–80}

A turbulent state of another kind has been obtained in the same geometry but with a wedge-shaped cell and an electric field applied. Well below the threshold for the instabilities described above one observes a turbulent motion⁸¹ of umbilics which are the defects of the order-parameter field for the Fredericks transition in homeotropic geometry. ⁸² This phenomenon has been described in terms of phase slippage of the super-conducting order-parameter^{79,81} and has lead to a theory of strong turbulence in nematics. ⁸³

VI CONCLUSION FOR PART I.

In this first part we have reviewed some selected experiments which lead to turbulence. This problem is much less advanced for nematics than for isotropic liquids. Some basic instability mechanisms are known. In many circumstances the presence of a director field does not change things very much in theory, except that the anisotropy removes degeneracy to a large extent. A consequence is that certain instability modes linked to rotational invariance may be hindered at given steps of the cascade. Convective structures tend to be rather regular and defects such as dislocations of rolls can be studied carefully. Simple optical observations are quite easy and informative for this general problem. The growth of spatial chaos in Electrohydrodynamic instabilities and the elliptical shear experiment is of special interest in comparison with Rayleigh-Bénard instability in extended geometry for isotropic liquids. Finally the possibility of topological defects in the director field seems to be the only truly original feature of nematics. To this respect they present themselves rather like superfluid Helium, i.e. good examples of ordered media susceptible to special kinds of turbulence. This possibility which has already been explored⁸² is further examined in the part II for the case of a shear flow experiment with $\alpha_3 > 0$ and the director parallel to the plane of velocities.

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Part II: On the Transition to Turbulence Via "Tumbling"

In Part I of this article we have pointed out that flow experiments in a nematic with viscosity coefficient $\alpha_3 > 0$ and initially aligned along the direction of flow could provide a nearly direct transition from laminar flow to turbulence original and specific of nematics. Turbulence here would result from continuous nucleation and annihilation of disclination lines with a more or less erratic motion; this process could occur after a tumbling of the director due to the fact that when $\alpha_3 > 0$, the nematic does not orient itself in a strong shear flow. In section I we recall the expression of the Leslie-Ericksen equations which account for a flow where the director remains in the plane defined by the velocity gradient. Except when making drastic simplifying assumptions, solutions cannot be obtained analytically when $\alpha_3 > 0$ under strong shear so we have developed a numerical solution able to manage with transients or with an eventual time dependence. The method is presented in § II. Results are given for simple shear flow in § III. Tumbling is described in details. Only time-independent solutions have been obtained. A remarkable fact is the first order like character of the transition with the coexistence of two solutions, one with a small distortion and the other with a large one, over a certain range of shearing rates. Dynamical aspects of tumbling are briefly examined. The experimental situation is summarized at the beginning of section IV. It strongly suggests to examine the role of disclinations of integer strength as well as other defects. The law governing the motion of such defects in a distorted medium is derived next. Finally we present some conjectures on the turbulent state that could exist due to a random motion of these orientation defects above the threshold for tumbling.

I THE ERIKSEN-LESLIE EQUATIONS

For simplicity we consider a simple shear flow experiment with strong anchoring conditions. Let x be the direction of the flow and z the normal to the moving plates which create the shear. The plates are parallel at a distance d from each other, the upper one sliding at a velocity V relative to the lower one which is assumed at rest

Equations governing the coupled fields θ and u are well known. In dimensionless form, they read:

torque equation:

$$\dot{\theta} = (1 - \delta \cos 2\theta)\theta'' + \delta \sin 2\theta \ \theta'^2 - \frac{u'}{2} (1 + \lambda \cos 2\theta) \tag{1}$$

force equation:

$$\zeta \dot{u} = \frac{\partial}{\partial z} \left\{ (\eta + \frac{\lambda}{2} \cos 2\theta + \frac{\epsilon}{4} \sin^2 2\theta) \ u' + \frac{1}{2} (1 + \lambda \cos 2\theta) \ \dot{\theta} \right\}$$
 (2)

where and denote time and space derivative respectively.

The distance d between the plates is the natural length scale. $T_0 = \gamma_1 d^2 / \bar{K}[(\bar{K} = 1/2(K_1 + K_3))]$ is the time scale as usual. The velocity scale is $V_0 = d/T_0$; V/V_0 is the Ericksen number of the flow. Other coefficients are reduced viscoelastic parameters of the nematic: K_i and α_i being the Frank constants and the Leslie viscosities respectively, we define:

$$\delta = (K_3 - K_1)/(K_3 + K_1)$$
 which measures the elastic anisotropy

 $\lambda = \gamma_2/\gamma_1 = (\alpha_2 + \alpha_3)/(\alpha_3 - \alpha_2)$ which is negative but may be of mudulus smaller or larger than 1.

 α_2 being negative, when α_3 is negative $|\lambda|$ is larger than 1 and at the limit of strong shears the nematic orients itself in the flow at the Leslie angle θ_L given by

$$\cos 2\theta_L = -\frac{1}{\lambda},$$

when α_3 is positive, the Leslie angle no longer exists and it is precisely the situation we are interested in.

Remaining parameters are:

$$\eta = (\eta_2 + \eta_1)/2\gamma_1$$
, $\epsilon = \alpha_1/\gamma_1$ and $\zeta = \rho \bar{K}/\gamma_1^2$

 η is ordinarily of the order of 1 (0.82 for MBBA) and ϵ is small ($\sim 8.4 \times 10^{-2}$ for MBBA).

 $\zeta = \rho \bar{K}/\gamma_1^2$ is very small, of the order of 10^{-6} it can be seen as the ratio of the characteristic time for damping of velocity fluctuation T_v to the corresponding quantity for orientation fluctuations T_0 ($\zeta \sim 10^{-6}$ for MBBA).

II THE NUMERICAL SOLUTION

The goal of our calculation is to mimic a shear flow experiment as closely as possible. Except making drastic simplifying assumptions² an analytic solution is out of reach and we have to turn to a numerical solution. Since it is not clear whether Eqs. (1, 2) can have time dependent solutions, it is interesting not to concentrate oneself on stationary solutions ($\dot{\theta} = \dot{u} = 0$) but to take time derivatives into account and to solve the complete initial and boundary value problem. Then Eqs. (1, 2) are replaced by difference equations after time-

space discretization. Let supercript n be the time index and subcripts i, j the space indices; with τ the time increment the simplest scheme would be

$$\theta_i^{n+1} = \theta_i^n + \tau \ F(\theta_i^n; \ u_i^n) \tag{3}$$

$$u_i^{n+1} = u_i^n + \tau \ G(\theta_i^n; \ \theta_i^{n-1}; \ u_i^n)$$
 (4)

it is called "explicit" since (θ, u) at step n+1 are univoquely and explicitly determined by (θ, u) at previous steps. However it is very badly "conditioned" since it involves two physical time scales T_0 and T_v of very different orders of magnitude. $(\zeta = T_v/T_0 \sim 10^{-6})$; in order to describe accurately the rapid velocity fluctuations one should choose $\tau \ll T_v$ which would forbid to describe the dynamics of orientation for obvious practical reasons. Since we are interested only in the part of velocity fluctuations which is "slaved" to orientation fluctuations we can neglect velocity fluctuations which evolve much faster i.e. assume $u_j^{n+1} = u_j^n$ in (4). So we have to solve u_i^n at given $(\theta_i^n, \theta_i^{n-1})$. This is indeed possible since it turns out that the problem for u^n is a linear one; moreover the matrix to be inverted is tridiagonal so that this is performed by Gauss elimination very efficiently even for very large systems (i.e. a very refined spatial mesh).

Once u^n is known, we have to turn to the determination of θ^{n+1} . At this point a new difficulty arises: the problem of numerical stability. This problem is already present for the integration of the heat diffusion equation³ which is the simplest conceivable problem. Discretization of $\dot{\theta} = \theta^n$ gives:

$$(\theta_i^{n+1} - \theta_i^n)/\tau = (\theta_{i+1} - 2\theta_i + \theta_{i-1})/h^2$$

where the right hand side (r.h.s.) can be evaluated either at step n or step n+1 in the simplest numerical schemes. When the r.h.s. is evaluated at step n one has an "explicit" scheme giving immediately θ^{n+1} in function of θ^n

$$\theta_i^{n+1} = \theta_i^n + (\tau/h^2) (\theta_{i+1}^n - 2\theta_i^n + \theta_{i-1}^n)$$

which turns out to be unstable against numerical noise when $\tau/h^2 > 0.5$. Now when the r.h.s. is evaluated at step n + 1 one has:

$$-(\tau/h^2)\,\theta_{i+1}^{n+1}+\theta_i^{n+1}\,(1+2\tau/h^2)-(\tau/h^2)\,\theta_{i-1}^{n+1}=\theta_i^n$$

The scheme is called "implicit" since to get θ^{n+1} one has to invert a linear system. Of course this involves more computation but this is rewarding since it can be shown that the scheme is stable whatever the time step τ be. The matrix to be inverted is tridiagonal so the solution can be efficiently obtained by some simple variant of Gauss elimination.

Numerical stability criteria are not known in the present non-linear problem but the highest spatial derivative remains the most "dangerous" term and one can expect a stability condition of the form $\tau/h^2 < \alpha$. Empirically one finds that $\alpha \approx 0.5$ as for the linear problem. This condition impedes to go to a

very refined spatial mesh without slowing down the evolution exaggerately. To get rid of this difficulty we have assumed $K_1 = K_3$ and thus $\delta = 0$ which greatly simplify the terms containing spatial derivatives of θ since ${\theta'}^2$ disappears and Eq. (2) reduces to the heat diffusion equation with a forcing term which can be solved using an implicit scheme. To summarize, the numerical solution involves two approximations; the first one concerns the response to rapid velocity fluctuations and seems quite legitimate; the second one is more questionable since it eliminates a term which certainly plays a rôle in the dynamics of the orientation. However if we limit ourselves to the vicinity of the temperature where α_3 changes its sign, i.e. far enough from the transition Nematic \rightarrow Smectic (N-Sm) if any, we expect K_1 and K_3 to be of the same order $(K_1 = K_3 = 2K_2)$ is a frequent approximation beyond the isotropic elasticity approximation). This would no longer be the case too close to the N-Sm transition⁴ since K_2 and K_3 diverge while K_1 remains finite (in the same way α_1 , α_3 and α_6 , γ_1 and η_1 diverge while α_2 , α_4 and α_5 , η_2 and η_4 remain finite). To take all terms into account one has either to return to the explicit scheme with its stringent stability condition or to develop an implicit scheme via a quasilinearization of the equations. We have avoided this last cumbersome analysis leaving it for future work since we think that most of the physics remains even assuming $K_1 = K_3$ or $\delta = 0$.

III NUMERICAL RESULTS

The numerical procedure is straightforward. At time t=0 one assumes a fluid at rest u=0 and oriented in the bulk uniformity at an angle θ imposed by boundary conditions. The number of points N in the z-direction was 20, 50 or 100 according to the precision required for an accurate description of region where θ and u evolve rapidly in space. The time step τ was not restricted by numerical stability requirement but was chosen in consideration of the evolution time of the solution, usually 1% of the natural time T_0 (\equiv 1 in dimensionless form), but smaller when the director "tumbled" (see below) or larger when θ and u approach a steady solution. Other parameters were $\eta=0.85$, $\lambda=-0.90$ and $\epsilon=0$; $\lambda=-0.90$ corresponds to $\alpha_3\cong |\alpha_2|/20$.

At step n, u is given by a system of the form:

$$A_{-}(\theta_{j}^{n}) u_{i-1}^{n} + A_{0}(\theta_{j}^{n}) u_{i}^{n} + A_{+}(\theta_{j}^{n}) u_{i+1}^{n} = G_{1}(\theta_{j}^{n}, \theta_{j}^{n-1})$$
for $i = 1, \ldots, N-1$.

and $u_0^n = 0$, $u_N^n = V$, θ at step n and n - 1 appears explicitly since we take into account the term $\dot{\theta} \simeq (\theta^n - \theta^{n-1})/\tau$ in Eq. (2). Then, at step n + 1, θ is given by

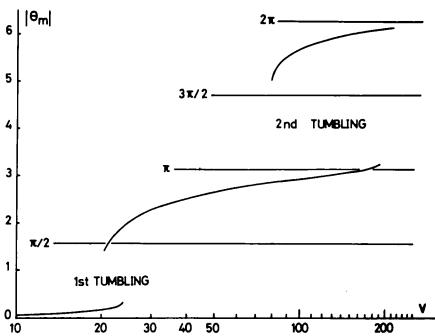


FIGURE 1 Tumbling is the sudden discontinuity of about $\pi/2$ in the curve giving the maximum θ_m of the angle θ the director makes with the x-axis as a function of the velocity V of the upper plate relative to the lower one. In all that follows V has been taken positive so that θ has negative values. Note the coexistence of two solutions which makes the tumbling 1st-order like in the terminology of phase transitions.

a system:

$$-\frac{\tau}{h^2}\,\theta_{i-1}^{n+1} + (1 + \frac{2\tau}{h^2})\,\theta_i^{n+1} - \frac{\tau}{h^2}\,\theta_{i+1}^{n+1} = \theta_i^n + \tau F_1\,(\theta_j^n, u_{j+1}^n, u_{j-1}^n)$$
for $i = 1, \ldots, N-1$

and $\theta_0^n = \theta_N^n = \theta$ at the boundaries. Our results are best vizualized by a series of figures.

Figure 1 displays the maximum of the orientation deformation as a function of the velocity V imposed at the upper plate in the case of planar anchoring ($\theta=0$). The first tumbling occurs between V=20.5 and 24 in good agreement with the analytical prediction of Pikin⁵ ($V\simeq22$ for $\lambda=-0.9$). The important point to be noted and which is worth experimental check is the coexistence of two solutions in a certain parameter range. This fact could be anticipated from the theory of the first order phase transitions between phases without mutual symmetry relation, according to the analogy between instabilities and phase transitions. Tumbling is the discontinuity of about $\pi/2$ be-

tween the two branches of the curve. Figure 2 displays the aspect of the two possible solutions at V=22. They are obtained with equal ease by numerical means while the expansion made to obtain an analytic solution⁵ impeded to get the strongly distorted one, which could lead to the uncomfortable feeling that there was no solution to all, both stationary and independent of transversal coordinates x and y. As can be seen from Figure 2 the deviations from the linear velocity profile expected in a simple shear flow remain quite small proportionally. Figure 3 displays the deformation for increasing shears. In order to visualize the deformation after the "tumbling" critical shear we have chosen the positions of points in the layer where $\theta = \pi/2$. This roughly corresponds to "tumbling lines" defined by Cladis and Torza (C-T) in Ref. 7. Here also we find that tumbling lines approach the plates when the shear is increased (Figure 4). At high shears the velocity profile becomes more complicated but only slightly differs from the linear one (see Ref. 6).

A second tumbling occurs between $V \cong 77$ and $V \cong 195$. The coexistence range is much larger than for the first one. This 2^{nd} tumbling is not likely to be observed since the deformation is very strong and the director is expected to escape in the transversal direction y in order to minimize elastic energy (see below §II).

The dynamics of the tumbling is qualitatively reproduced in Figure 5 which displays the evolution of the maximum θ_{max} of the distorsion as a function of time and gives photographs of θ and u taken at equal time intervals $\Delta t = 0.25$, the time step τ being 2.5×10^{-3} and the number of points along z N = 50 in the experiment; the starting point was the stationary state at V = 23.75 and V was suddenly increased to V = 24. (To give an idea of the precision and the role of time truncature errors, a simulation with $\tau = 10^{-2}$

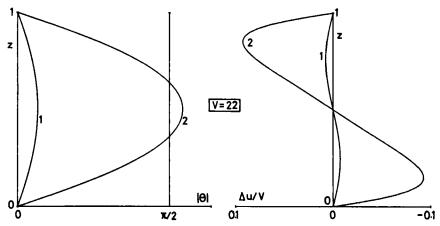


FIGURE 2 Aspect of the 2 possible solutions (1 and 2) at V = 22. Δu denotes the difference between the actual velocity u and the linear profile typical of simple shear in isotropic liquids.

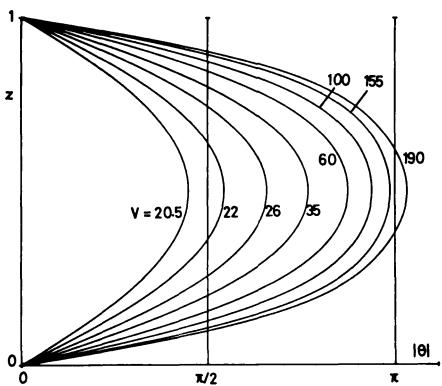


FIGURE 3 Growth of the distortion in the tumbled state as a function of the velocity V. The maximum θ_m has already been given in Figure 1. Velocity deviations have a rather complicated profile but they have been found smaller than 10% in all circumstances.

gives exactly the same evolution but with a time lag of 5-10% of the elapsed time).

IV DISCUSSION AND CONJECTURES

In this section we shall give more details on the experimental results obtained so far. The final purpose will be to interpret Gähwiller's findings of a turbulent state in HBAB Poiseuille flow when α_3 is positive. As can be seen from Figure 3, the "tumbled" state stores a great deal of Splay Bend elastic energy and the director can be tempted to escape in the transversal direction thus creating twist and lowering Frank energy since usually $K_2 < K_3$, K_1 . As observed by Pieranski, "disclination lines" can nucleate in the flow separating region where elastic energy has partly relaxed from regions where it has not. These and similar defects are expected to play an important rôle in the dynamics of the turbulent state observed by Gähwiller. By a dimensional argument we

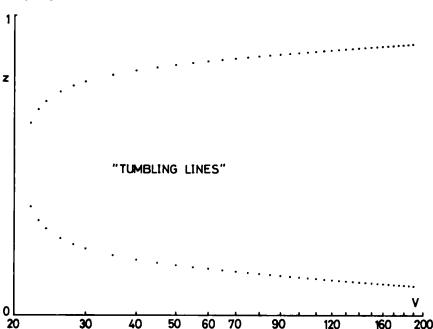
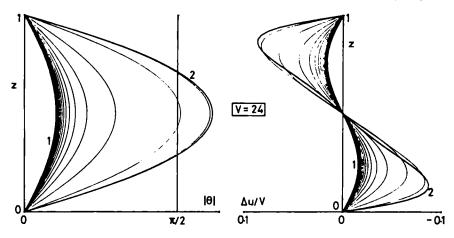


FIGURE 4 The ordinate of the points where $|\theta| = \pi/2$ is used to characterize the deformation of the tumbled configuration, this roughly corresponds to the tumbling lines observed by Cladis and Torza.

shall derive the law of motion of such defects and extend the result as a conjecture on the spatio-temporal behavior of turbulence by repeated tumbling.

Short review of the experimental situation

Before the experiment of Gähwiller, 8 the existence of nematics which do not align in a shear flow (i.e. with $\alpha_3 > 0$) was not suspected. Using nematic HBAB and a Poiseuille flow geometry he discovered a temperature domain where instead of an alignment the angle of which leads to the determination of α_3/α_2 , he found a non-stationary situation: "As the temperature is lowered past this critical point, the flow turns abruptly from a uniform configuration into many irregular rotating domains over the entire volume." Later, Pieranski and Guyon⁹ (P-G) performed careful optical measurements at low shearing rates in a simple shear flow geometry. They confirmed the existence of a regime with $\alpha_3 > 0$ in HBAB and concerning the high shear regime they observed a tendency for the molecules to get out of the plane of velocities at right angle with the direction of the flow. Similar experiments were undertaken by Cladis and Torza (C-T)^{6,7} in cylindrical Couette geometry but conducted in order to detect a Taylor type instability. As already noted they did observe tumbling but some obscure points remained about the director con-



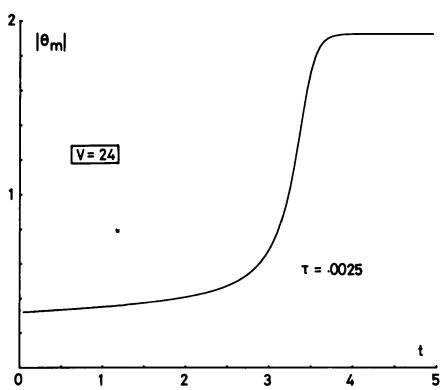


FIGURE 5 "Dynamics" of tumbling: the initial state (1) is the time independent configuration obtained at V = 23.75 at the upper limit of the existence range of the small deformation state. A "photograph" is taken every time interval $\Delta t = 0.25$ (upper part). The evolution of θ_m with time is given in the lower part.

figuration in boundary layers and the nature of the secondary instability, which lead P-G to question their interpretation. Despite the differences in geometry (cylindrical) and boundary conditions (homeotropic) we think that our numerical results presented in section III bring some support to Cladis-Torza's interpretation in terms of "tumbling" and tend to restrict the significance of Pieranski-Guyon criticisms. 10

If deformations up to the first tumbling have been found in agreement¹¹ with theoretical predictions of Pikin,⁵ it seems that several configurations are possible above the tumbling threshold. Besides the tumbled state observed by Cladis and Torza one can find cases where the director is nearly at right angle with the flow⁹ (in the y-direction) or more complicated situations¹¹ with regions where the director has turned by 2π around the normal to the plates inserted in regions where it has not, boundaries taking the form of thick 2π -disclination lines roughly parallel to the direction of the flow.

2 Discussion: generation and motion of "defects".

Consider first Figure 3 which displays the distortion θ in the time independent configuration where the director has "tumbled". As one can easily understand such a strongly distorted state can survive only if it is stable against fluctuations which make the director turn out of the xOz plane. A stability analysis has been developed by Pieranski-Guyon and Pikin¹¹ below the tumbling threshold; their conclusion was that an asymmetrical instability making the director leave the xOz plane was masked by the symmetrical one where n remains in the xOz plane (i.e. tumbling that they called the "water-mill" instability mode). A similar result for the case above the tumbling threshold has not yet been obtained. If one neglects the contribution of shears, one easily realizes that the nematic should like to replace the high amount of Splay-Bend distortion in the "tumbled" state (Figure 3) by some Twist deformation, which would lower the elastic energy content of the flow since usually $K_2 < K_1 \sim K_3$.

A first possibility is the nucleation of 2π twisted regions bounded by thick disclination lines. The situation pictured in Figure 6a is strongly reminiscent of that described by Stieb and Labes¹² for their generation process of integer strength disclinations. On the left the director is in the "tumbled" configuration, on the right it is twisted and the 2π -line separates the two regions. Such lines come in by pairs, the second member of which can be deduced easily. As long as the shear is maintained, since the elastic energy is partially relaxed in the twisted region, disclination lines should move in the direction of non-twisted regions (Figure 6a). When the shear is suppressed, in the region where the director is still in the xOz plane the distortion induced by the shear disappears rapidly and the orientation becomes uniform which cannot be the case in the twisted region (Figure 6b). The situation is reversed and uniform region grows at the expense of the twisted region: the line migrates in the reverse direction. Such defects and their migration has been observed by P. Pieranski. ¹³

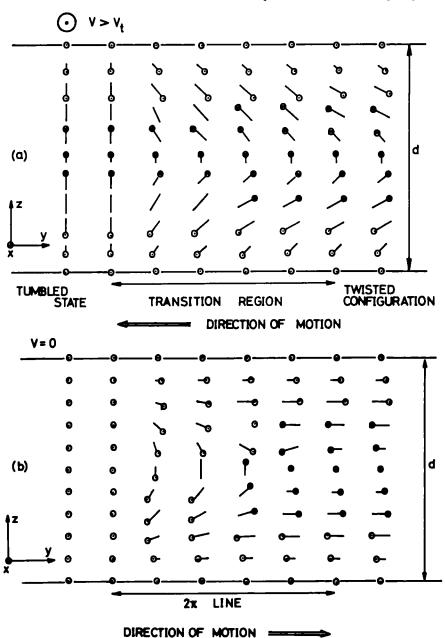


FIGURE 6 Nucleation of a 2π -twisted configuration: under shear (a) the director tends to escape laterally creating a 2π -twisted region. The transition region moves leftwards in order to lower elastic energy. After the shear has been suppressed (b) the director tumbles back towards the uniform configuration on the left and the transition region evolves naturally towards the 2π -disclination line which must propagate towards the right. Such lines have been observed by P. Pieranski.¹³

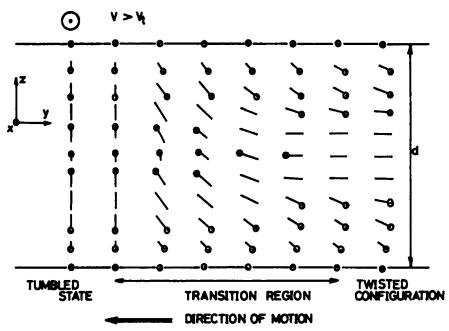


FIGURE 7 Nucleation of a $\pi/2$ twisted configuration occurs when the director escape transversally in the same direction both in the upper and lower parts of the cell. The $\pi/2$ -wall thus produced moves on the left. $\pi/2$ twisted region with the director at right angle with the velocity and velocity gradient have been observed by Pieranski and Guyon.

The velocity has been found inversely proportional to the thickness d, a feature that we shall derive below by a dimensional argument.

Another possibility is the nucleation of a region where the director is at right angle with the velocity and the velocity gradient. This is pictured in Figure 7. The director now rotates in the same direction in the upper and lower half of the flow whereas in the previous case it was rotating in opposite directions. As before the transition regions (walls) come in by pairs which cannot stay at rest but are expected to separate from each other more and more.

Up to now the rôle of shear has been taken into account only through the fact that it makes the director tumble. One should also consider its effects on the configurations resulting from the nucleation processes sketched above. Qualitatively they can be understood in terms of viscous torques exerted on the director simply adapting the approaches developed in Ref. 11 or 18. For example when the director has been brought along the (transversal) y-direction (Figure 7), viscous torques act to maintain n in that direction as long as the shearing rate is lower than a certain threshold above which an instability in form of a periodic distortion takes place. (Pieranski-Guyon instability when $\alpha_3 > 0$). In the same way viscous torques tend to stabilize the central layer of the twisted configuration at the right of Figure 6a as long as $-\pi < \theta < -\pi/2$.

This is no longer the case when $\theta < -\pi$ (i.e., in competition with the second tumbling see Figure 1).

Energy barriers for the nucleation of the two types of twisted states may be very dependent on the exact value of the viscoelastic constants, which would explain the somewhat incompatible findings reported in the literature.

In the simple shear flow case, it seems that the final state is time independent at least at not too high shearing rates. 7,11 The reason is probably that strong anchoring at boundaries and (approximately) constant shearing rate put too stringent symmetry conditions on the possible configurations, forbidding a random motion of defects. In the Poiseuille flow case the situation is profoundly different since the shearing rate is strongly varying along the thick ness of the cell (z-direction), reversing its sign at midway. Thus the flow can be decomposed into three layers. The central layer is rather "neutral" since the shear is quite weak. On the contrary, in the two layers close to the upper and lower plates, the shear is strong and variable thus strongly affecting the tumbling threshold. Moreover, each active layer has rather unsymmetrical boundary conditions since anchoring is strong at the plates while the central layers play more or less the rôle of a soft anchoring. Existence of an irregular motion of domains is thus very plausible since the exact configuration of the director will depend on fine details of two weakly interacting subsystems (the two "active" layers) where the tumbling threshold is position dependent and where several kinds of structure can nucleate at more or less random positions. It may be that intermediary time independent or time periodic states exist for a limited range of flow rates but chaos should appear very soon. Permanent erratic motion of "rotating domains" would come from repeated tumbling, creation and annihilation of defects. Statistical properties of that turbulent state are conjectured at the end of the next section which is devoted to the determination of the law of motion of disclination lines observed by Pieranski.

3 Motion of defects

Let us concentrate ourselves on the motion of a disclination line as observed by Pieranski after the suppression of the shear. As already stated the line which separates the region where the director is uniform from the region where it is twisted moves in the direction of the non-relaxed twisted region. Its velocity is obtained by a very simple dimensional argument which states that when the permanent regime is reached elastic energy released by the displacement is converted in heat through viscous process. (This is very similar to the case of walls¹⁶ or umbilics¹⁷ for the Freedericks transition in homeotropic geometry).

Elastic estimate: the energy gained in making a length l of line displaced on a distance equal to its diameter \emptyset is

$$\Delta E \sim \Delta K (\nabla n)^2 \times (\text{vol})$$

where $|\nabla \mathbf{n}| \sim \Delta \varphi / \emptyset$, $\Delta \varphi$ being a rough measure of the angular variation in-

volved, the diameter \emptyset giving the order of magnitude of the distances over which this variation takes place. Since the line is thick with thickness $\emptyset \sim d$ one has

$$\Delta E \sim \Delta K \times (\Delta \varphi/d)^2$$
 [vol = (length l) × (height = d) × (width = d)]

Dissipation estimate: the dissipation by unit time and unit volume Σ is given by

$$\Sigma \sim \gamma \times (\dot{\mathbf{n}})^2$$

where γ is an averaged rotational and $|\dot{\mathbf{n}}| \sim \Delta \varphi / \Delta t$, Δt being the time it takes to make the director rotate.

Velocity of the line: let v be the velocity we are looking for. When the director has turned by $\Delta \varphi$ this means that the line has passed at the point considered; the process occurs on a distance $\emptyset \sim d$; the time required is $\Delta t = d/v$ so that one has:

$$\Delta E \sim \Delta K \times (\Delta \varphi/d)^2 \times (\text{vol}) \sim \Sigma \times \Delta t \times (\text{vol})$$

 $\sim \gamma \times (\Delta \varphi/\Delta t)^2 \times \Delta t \times (\text{vol})$

which simplifies as:

$$\Delta K/d^2 \sim \gamma/\Delta t \tag{5}$$

or using the relation with v:

$$v \sim \Delta K/\gamma d$$

i.e., v inversely proportional to the thickness as experimentally observed. Motion of the "defects" generated by the nucleation of twisted regions should follow a similar law for dimensional reasons. Now let us derive some statistical properties of the turbulent state in the Poiseuille flow.

First assume the free motion of n pairs by unit length in the transversal direction y (n behaves as a wave number). According to the argument developed above their velocity is known. Pairs thus created can propagate only on a distance of the order of 1/n before annihilating with neighboring pairs, thus it takes a time ΔT_a

$$\Delta T_a \sim 1/vn$$

to annihilate all the pairs.

After annihilation the nematic is ready for a new tumbling, the distortion grows according to

$$\gamma \dot{\theta} \sim$$
 (externally applied torque = viscous shear torque).

The viscous torque is of the form $\sigma_{\rm vis} \sim \alpha \bar{s}$ where α is a viscous torque coefficient and \bar{s} some average value of the shearing rate (proportional to the pres-

sure gradient driving the flow). The growth time ΔT_g is then of the form:

$$\Delta T_g \sim \gamma/\alpha \bar{s} \sim 1/\bar{s}$$

In permanent regime one should have

$$\Delta T_a \sim \Delta T_g$$

so that:

$$\frac{1}{n} \sim \frac{1}{s} \text{ or } n \sim \bar{s}/v \tag{6}$$

(Due to the relation giving v one can see that in this regime the viscous shear torque $\alpha \bar{s}$ the orientational damping rate $\gamma \theta$ and the elastic contribution $K\theta''$ omitted above are all of the same order of magnitude).

From (5,6) one deduces that the width of the rotating demains should vary as $1/n \sim v/\bar{s} \sim \Delta K/\gamma d\bar{s}$. In fact the size of defects and thus their velocity may vary with the shearing rate, the channel being sliced into two "active" layers where the shear is strong and a more or less "neutral" layer in the center where the shear is weak. The typical transversal dimensions \emptyset of the defects being linked to the effective thickness of the "active" layers $(\emptyset \sim \delta)$ moreover one can think of an asymptotic regime of a dense network of defects where the distance between defects would be of the order of their dimensions so that $n \sim 1/\delta$, which leads to

$$\delta \sim \Delta K/\gamma \delta \bar{s}$$

or

$$\delta \sim 1/\sqrt{\bar{s}}$$

the time associated with this length scale being $\sim 1/\bar{s}$. A similar approach was first introduced by Katz and Volovik¹⁴ for the problem of the erratic motion of disclination lines in a nematic submitted to a circular shear in planar geometry using an analogy with the turbulence in superfluid helium.¹⁵

V CONCLUSION FOR PART II

In this second part we have studied in details the tumbling phenomena observed by Cladis and Torza.^{6,7} The first point we want to stress is that when things seem too complicated to be described reliably by current approximations, one should not hesitate to perform a numerical simulation directly on the primitive equations. We think that the numerical solution obtained above the threshold clarify a somewhat obscure controversy^{10,11} in the sense that it gives explicitly the form of the distortion above the tumbling threshold and

can also give reliable information on the process which leads to it. The main problem of this approach is that of numerical stability; it may be turned here if one accept certain approximations. However, the situation may become very intricate when one deals with more than one spatial dimension.³

The second point follows from section IV. Clearly much work remains to be done for a clear understanding of the kind of turbulence observed by Gähwiller. In our opinion, progress should come from a study of the dynamical process of defect generation-annihilation and the coupling with flow variables. This transition to turbulence where the order parameter plays a crucial rôle is quite original and obviously require new experiments and further theoretical developments which could come and confirm or contradict our conjectures. ¹⁹

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