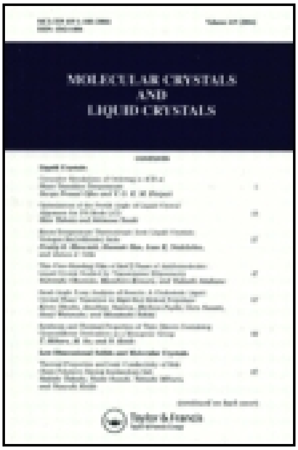

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Smectics: A Model for Dynamical Systems ?

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SMECTICS : A MODEL FOR DYNAMICAL SYSTEMS ?

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Abstract The dynamics of the structure (rolls and dislocations) appearing in some dynamical systems (instability above a threshold) is given by analogy with the hydrodynamic description of Smectic Liquid Crystals.

INTRODUCTION

In many nonequilibrium systems there exists, above a threshold value of some control parameter, a transition from a homogeneous state to an organized structure. Very often the first observed state corresponds to straight rolls (as in the classical Rayleigh Bénard convection) see fig. 1. Experiments in "large boxes" (large aspect ratio) do show as well slow spatial variation of the roll structure (compression, dilatation and change in the orientation of the rolls) as dislocation like defects. In what follows we shall not be concerned with a complete hydrodynamic description of phenomena. The precise knowledge of the mechanisms at the origin of the observed instabilities will be left aside. We shall focuss our attention to the dynamics of the order parameter, characteristic of the symmetry breaking occurring at the transition (threshold of the instability). The breaking of translational symmetry in one direction of space (roll structure) is similar to the one present in smectics (layered systems).[1] In "large box" samples with a large number of rolls, a homogeneous translation of the rolls will relax infinitely slowly. The phase variable ϕ which describes the position of the rolls is then a hydrodynamical variable equivalent to the position u of the Smectic layers. The purpose of this article is to illustrate on a few exemples issue from ref. 2 and 3 how the use of the Smectic analogy allows to understand the phase dynamics in these systems. In particular, we will show that the elliptic shear induced roll instability in Nematics is analogous to Smectics C and that a wedge is analogous to a temperature gradient. Indeed in that case the symmetry of the system is similar to the one of Smectics C (the direction of horizontal flow is not perpendicular to the axis of the rolls). We shall now give a general outline of the main points already developed in refs. 2 and 3.

PHASE DYNAMIC EQUATION

The dynamics of the phase ϕ is described by analogy with the well known dynamical behavior of Smectics close to equilibrium.[4] Let us define the roll size as $a_o = 2\pi/q_o$ and the phase $\phi = - q_o u$ where u is the displacement (as in Smectics) of the layers (see fig. 1). The precise form of the elastic free energy F depends on the type of the instability considered. For instabilities in which the wave vector, at threshold, is degenerate (no preferred direction of the rolls) a Smectic-like elastic free energy gives a good description of bend or compression of the layers. Contrary an elasticity of a 2D-solid type describes systems where the direction of the rolls is fixed.

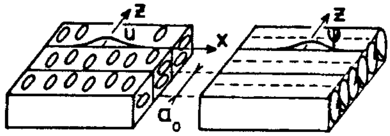

FIGURE 1. Analogy between Smectics layers a) and convective rolls b)

This happens for example in the case of an elliptical shear excitation and we define

$$F= \frac{1}{2}\int dxdz \{B_{\parallel} (\frac{\partial \phi}{\partial z})^2 + B_{\perp} (\frac{\partial \phi}{\partial x})^2 + \text{Higher order terms.}\} \quad (1)$$

In what follows all lengths are scaled by q_o. Although our analysis is valid for all type of roll instabilities, we restrict our examples to the elliptical shear instability (after referred as E.S.I.) where experiments have been performed.

Since in far from equilibrium situations we are here only concerned with the description of the macroscopic structure the velocity field $\underset{\sim}{v}$ corresponds to an average value (over the sample thickness). The corresponding effective "Navier-Stokes " equations will then depend on boundary conditions. Indeed for rigid-rigid (R-R) boundary conditions the y dependence of velocity fluctuations implies modes with wave vectors $q_y \sim \pi/d_o$ (d_o is the sample thickness) and on the contrary to possible modes $q_y = 0$ in the case of free-free (F-F) boundary conditions. This leads to the effective hydrodynamic equations :

$$\rho\frac{\partial V_i}{\partial t} = - q_o \nabla_i P + q_o^2 (\frac{\delta F}{\delta \phi}) \delta_{iz} - \zeta_i V_i \qquad (2)$$

where $\zeta_i = \eta q_o^2$ corresponds to a Darcy flow for R-R boundary conditions and $\zeta_i = \eta\Delta$ for F-F boundary conditions

$\frac{\partial V_x}{\partial x} + \frac{\partial V_z}{\partial z} = 0$ is the incompressibility condition (3)

The main point of a Smectic-like description is the natural introduction of the coupling to the vertical vorticity, already present in the permeation equation (the permeation strength is defined by the parameter λ_p) :

$$\frac{\partial \phi}{\partial t} + V_z = - \lambda_p q_o^2 \frac{\delta F}{\delta \phi} \qquad (4)$$

which was neglected in classical amplitude equations.[6] Originally, amplitude equations valid for large system close to threshold described the dynamics of slow modulations of the structure. These equations, as well as the phase equation introduced later[7] derived from a variational principle and only accounted for relaxational behaviors. The introduction of the permeation (eq. 4) brakes this potential behavior. This was already pointed out in a different way in the second paper of Siggia and Zippelius[8] who found that the relaxational equation for the amplitude was seriously in error for free-slip boundary conditions and finite Prandtl number. They noticed the importance of the coupling to the vertical vorticity leading to non variational behavior. Our description takes into account the coupling between a large scale flow and the structure motion or deformation. A recent analysis[9] shows precisely how the presence of long-wavelength vertical vorticity leads to such a drift term correcting the classical phase equation and playing an important rôle in the instabilities of straight rolls near onset.

Using eq. 3, the pressure is eliminated in eq. 2 and one obtains, coupled to eq. 4, the general dynamical phase equation :

$$\rho \frac{d}{dt} (\Delta V_z) = q_o^2 \frac{\partial^2}{\partial x^2} \frac{\delta F}{\delta \phi} + (\zeta_{/\!/} \frac{\partial^2}{\partial x^2} + \zeta_\perp \frac{\partial^2}{\partial z^2}) V_z \tag{5}$$

It is worth noticing that in the case of strong permeation $\lambda_p \to \infty$, the flow of matter and the structure (position of the rolls) become independent. One recovers a classical, potential phase equation[7] :

$$\frac{\partial \phi}{\partial t} = - \lambda_p q_o^2 \frac{\partial F}{\partial \phi} \tag{6}$$

where in the case of the shear instability :

$$\frac{\partial F}{\partial \phi} = - (B_{/\!/} \frac{\partial^2 \phi}{\partial z^2} + B_\perp \frac{\partial^2 \phi}{\partial x^2}) + \ldots.. \tag{7}$$

Experiments[10] reveal dislocations moving at a uniform velocity $\underset{\sim}{V}_o$. Phase equations (5)(4) need to be modified in order to take into account singularities introduced by the presence of dislocations.

STRAIN PATTERN AND VELOCITY OF A MOVING DISLOCATION.

Dislocations moving with constant velocity $\underset{\sim}{V}_o$ correspond to solutions $\phi = \phi(\underset{\sim}{r} - \underset{\sim}{V}_o t)$ and $\underset{\sim}{v} = v(\underset{\sim}{r}_o - \underset{\sim}{V}_o t)$ which imply $\frac{\partial}{\partial t} = - \underset{\sim}{V}_o \cdot \underset{\sim}{\nabla}$ in dynamical equations. Dislocations induce singularities of the phase ϕ but not of the compression $\partial\phi/\partial z$ or of the tilt of the layers $\partial\phi/\partial x$, at least outside of their core (we follow the approach given in ref. 11). $\underset{\sim}{m}$ is a vector having for components tilt and compression. A positive ($\varepsilon_d = + 1$) edge dislocation corresponds to a density $\underset{\sim}{j}$:

$$\underset{\sim}{j} = \underset{\sim}{\nabla} \times \underset{\sim}{m} = \varepsilon_d \, 2\pi \, \delta_x \, \delta_y$$

and to a quantification for any circuit around it (fig. 2):

$$\int_c \underset{\sim}{m} \cdot \underset{\sim}{d\ell} = 2\pi \, \varepsilon_d$$

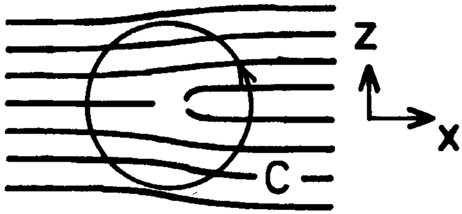

FIGURE 2. Positive ($\varepsilon_d = +1$) edge dislocation.

with these definitions the phase equations now reduce to the unique one :

$$(\zeta_{\parallel}\frac{\partial^2}{\partial x^2}+\zeta_{\perp}\frac{\partial^2}{\partial z^2})\underset{\sim}{V}_o\cdot\underset{\sim}{m}=-q_o^2\{(1+\lambda_p\zeta_{\parallel})\frac{\partial^2}{\partial x^2}+\lambda_p\zeta_{\perp}\frac{\partial^2}{\partial z^2}\}\underset{\sim}{\nabla}\cdot\underset{\sim}{\Phi}(\underset{\sim}{m}) \qquad (8)$$

where $\underset{\sim}{\nabla}\cdot\underset{\sim}{\Phi}$ stands for $-\frac{\delta F}{\delta\phi}$ and

$$\underset{\sim}{\Phi}(\underset{\sim}{m}) = B_{\parallel}\, m_z\, \underset{\sim}{z} + B_{\perp} m_x\, \underset{\sim}{x} \qquad (9)$$

for E.S.I. case (one has assumed a low velocity $\underset{\sim}{V}_o$ compared to the sound velocity). Inversion of the Fourier transformed solutions of eq. 8 gives the strain field around a moving dislocation $\underset{\sim}{m}(x,z)$. Solutions are given in ref. (2).

The main results are the following : the symmetry of distorted regions around a moving dislocation is modified compared to the static one. The z symmetry of the strain is broken by a glide velocity V_{oz} and the x symmetry by a climb velocity V_{ox}. There is a great difference between the front and the wake of the motion in the case of a pure glide or climb motion. The strain decreases exponentially in the front and with a power law in the wake of the motion. The screening length $\sim D/V_o$ defining the front of the motion allows to determine the phase diffusion coefficients $D_{\parallel,\perp} = \lambda_p\, q_o^2\, B_{\parallel,\perp}$. A fit between experimental and theoretical strain pattern around the moving dislocations gives an estimate of $D_{//} \sim 10^{-4}$ cm^2/s which is in agreement with theoretical estimate $D_{//} = \xi_o/\tau_o$ where τ_o and ξ_o are the slowest relaxation time and influence length close to threshold.

The relation between the motion of a dislocation and the external stress $\underset{\sim}{\Phi}^o$ is obtained from a momentum balance equation which at the end reads[2] :

$$\underset{\sim}{P} = -\int(\underset{\sim}{\Phi}^o \wedge \underset{\sim}{j})dv = -\int(\underset{\sim}{\Phi}^d.\underset{\sim}{\nabla})\underset{\sim}{m}^d \, dv \tag{10}$$

where $\underset{\sim}{\Phi}^d$ and $\underset{\sim}{m}^d$ are the stress and strain due to the dislocation. One recognizes in the left hand side of eq. 10 a typical Peach-Koehler force $\underset{\sim}{P}$ acting on dislocations in classical crystals[12]. The right hand part is estimated with use of the phase dynamical equation 8. This leads to the relations between the external stress and the dislocation velocity :

$$P_z = - \varepsilon_d \, \Phi_x^o = \lambda_{zz} V_{oz} \tag{11}$$

$$P_x = + \varepsilon_d \, \Phi_z^o = \lambda_{xx} V_{ox} \tag{12}$$

Expressions of "effective" viscosity coefficients λ_{ij} which already depend on dislocation velocity V_o lead to the following typical behaviors[2]:

- Smectics or F-F Rayleigh Bénard :

$$\left.\begin{matrix} V_{ox} \\ V_{oz} \end{matrix}\right\} \text{very small} \quad \lambda_{xx} \sim \text{const}$$

$$\begin{matrix} V_{ox} >> V_{oz} & \lambda_{xx} \sim V_{ox}^{-1/3} & \\ & & \lambda_{zz} \sim \text{const} \\ V_{oz} >> V_{ox} & \lambda_{xx} \sim V_{oz}^{-1/2} & \end{matrix}$$

- R-R Rayleigh Bénard :

$V_{ox} >> V_{oz}$ $\lambda_{xx} \sim V_{ox}^{-1/3}$

$V_{oz} >> V_{ox}$ $\lambda_{yy} \sim V_{oz}^{-1/2}$ $\lambda_{zz} \sim$ const

- E. S. I.

For all V_{ox}, V_{oz} : λ_{xx} and λ_{zz} are velocity dependent (exact values are given in ref. (2)). A typical behavior at low velocity is of the type $\underset{\sim}{P} \sim \underset{\sim}{V} \log (q_c D/V)$ where q_c is a typical short length scale.

For the crossover between the different regimes see ref. 2 . One recovers for a pure climb motion the Siggia-Zippelius law $P_x \sim V_{ox}^{2/3}$ for all velocities in the R-R case but one predicts a true viscosity $\lambda_{xx} \sim$ const. for law velocities in the F-F case. In all three cases the climb viscosity λ_{xx} is lowered by glide or climb motion.

DISLOCATIONS MOTION IN A WEDGE SAMPLE

Experiments have been performed[3] in wedged samples of angle θ and thickness $d = d_o + \underset{\sim}{r}.\underset{\sim}{\theta}$. Here we only consider a wedge of the type $\theta_z = \theta.z$ and focuss our attention to symmetry properties. The instability is induced by applying an elliptical shear (displacement of the upper plate of the form $x_E = x_o \sin \omega t$, $z_E = z_o \cos \omega t$ in a homeotropic nematic sample). The tilt direction of the wedge is adjusted in order to be perpendicular to the roll axis (Ox) (fig. 3). Nucleation, annihilation and motion of dislocations are observed. Nucleations of pairs of dislocations appear preferentially on a parallel to the equator (z ≃ const.).

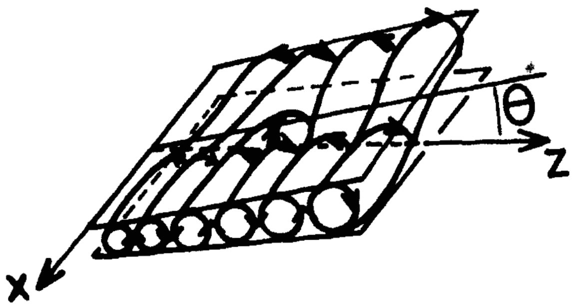

FIGURE 3. Wedge of angle $\underset{\sim}{\theta} = (0, \theta_z)$

Both glide and climb motions are observed. A schematic drawing of the defect motion of positive or negative sign ($\varepsilon_d = \pm 1$) is given in fig. 4.

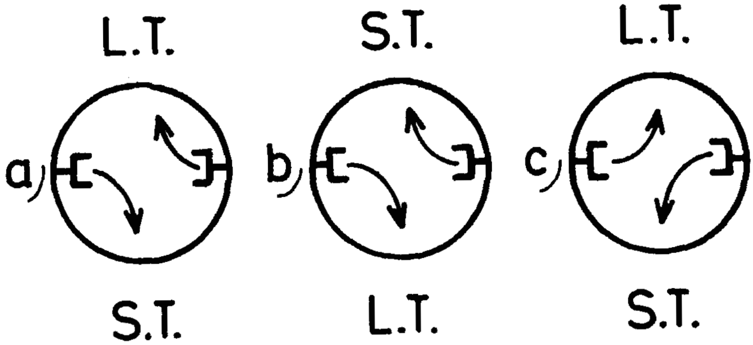

FIGURE 4. Schematic drawing of dislocation motion in a wedge
a) angle of the wedge θ and negative sense of rotation of the elliptical shear (E < 0)
b) angle of the wedge − θ and negative E
c) angle of the wedge θ and positive E
L.T. and S.T. mean large and small thickness

The sign of θ does not seem to affect dislocation motion. On the contrary, a change of the sense of the elliptical shear ($E \to -E$) induces a glide direction modification. A systematic study of the dislocation velocity $\underset{\sim}{V}_o$ versus the position in the whole cell has not been performed. Observation in a region close to the equator[3] indicates an increasing glide velocity V_{oz} but an essentially constant climb velocity V_{ox} as a function of an increasing wedge angle θ. The nature of the motion as a function of the sign of the elliptical shear indicates a Smectic C behavior. This behavior is already evidenced by the precise theoretical knowledge of the elliptical shear instability[5]. The direction of the rolls Ox appears at an angle α with the axis Ox_E of the excitation (fig. 5). This defines a direction equivalent to the director in a Smectic C.

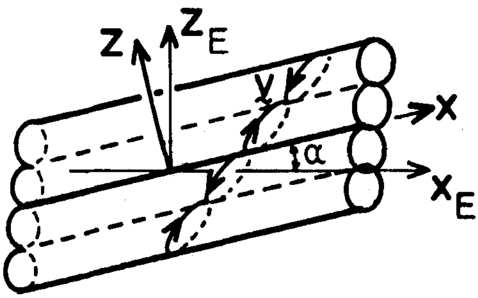

FIGURE 5. Flow direction in an elliptical shear instability.

The hydrodynamical velocity gets two non zero components V_x, V_z in the horizontal plane such that a change in the rotational sense of the elliptical excitation induces the change $\alpha \to -\alpha$ but also $(V_x . V_z) \to -(V_x . V_z)$. The free elastic energy is written taking into account the static coupling (term C in eq. 13) between the wedge and the roll structure the periodicity of which depends on the sample thickness. θ is equivalent to a thermal gradient ∇T in Smectics or in cholesterics which leads to the modification of the layer period.

$$F = \frac{1}{2}\int dx\,dz\,\Big(B_{/\!/}\,(\frac{\partial\phi}{\partial z})^2 + B_{\perp}\,(\frac{\partial\phi}{\partial x})^2 + 2C\,\delta d\,(\frac{\partial\phi}{\partial z})$$

$$+ 2C'\,\delta d\,(\frac{\partial\phi}{\partial x}) + 2E\,(\frac{\partial\phi}{\partial x})(\frac{\partial\phi}{\partial z})\Big) \qquad (13)$$

The last two terms are characteristic of a Smectic C structure. The elastic coefficient E changes its sign with the rotational sense of the elliptical shear. An estimate of coefficients C and C' is obtained[3] with use of properties of the system close to the instability threshold. One gets :

$$C' = E/\pi \qquad (14)$$

$$C = B\ /\pi \qquad (15)$$

In presence of a wedge the permeation equation now reads:

$$\frac{\partial\phi}{\partial t} + V_z = \lambda_p\, q_o^2\, \underset{\sim}{\nabla}.\underset{\sim}{\Phi} + q_o^2\, \xi_{/\!/}\, \theta_z + q_o^2\, \xi_{\perp}\, \theta_x \qquad (16)$$

where $\xi_{/\!/}$ and $\xi_{\perp}$ are respectively characteristic of a Smectic A and C. They are equivalent to the thermomechanical coupling in Cholesterics (Lehmann effect[13]) and Smectics and reminiscent of the Soret effect in binary mixtures.[4]

The precise form of the stress $\underset{\sim}{\Phi}^o$ depends strongly on experimental conditions. In fact in the largest thickness region experiments show that the system is subcritical : there is no stress on the rolls ($\Phi_x^o = \Phi_z^o = 0$ at $z = \pi L/a_o$). Furthermore one does not observe any large scale motion of the structure (no "macroscopic" flow other than that at the periodicity of the rolls) and compression, orientation of the rolls do not depend on x. All these features imply a stress field $\underset{\sim}{\Phi}^o$ of the form :

$$\Phi_x^o = B_{\perp}\,\frac{\partial\phi^o}{\partial x} + E\,\frac{\partial\phi^o}{\partial z} + C'\delta d \qquad (17)$$

$$\Phi_z^o = B_{/\!/} \frac{\partial \phi^o}{\partial z} + E \frac{\partial \phi^o}{\partial x} + C\ \delta d \qquad (18)$$

satisfying eq. 16, written with $V_x = V_y = \frac{\partial \phi}{\partial t} = 0$ (no "macroscopic" flow) :

$$\lambda_p \frac{\partial \Phi_z^o}{\partial z} = - \xi_{/\!/}\ \theta z$$

which leads, taking boundary conditions into account (assuming a rectangular cell between z = - L and z = + L), to :

$$\Phi_z^o = \xi_{/\!/} / \lambda_p\ \theta (\frac{\pi L}{a_o} - z) \qquad (19)$$

$$\Phi_x^o = \xi_{/\!/} / \lambda_p\ (\frac{E}{B_{/\!/}})\ \theta (\frac{\pi L}{a_o} - z) \quad \text{for a } \underline{\text{wedge} + \theta} \qquad (20)$$

and

$$\Phi_z^o = (\xi_{/\!/} / \lambda_p)\ \theta (z + \frac{\pi L}{a_o}) \qquad (21)$$

$$\Phi_x^o = (E/B_{/\!/})\ (\frac{\xi_{/\!/}}{\lambda_p})\ \theta (z + \frac{\pi L}{a_o}) \quad \text{for } \underline{\text{a wedge} - \theta} \qquad (22)$$

First notice that the "thermomechanical" coupling induces a stress linearly increasing with z. In a Smectic A only a stress Φ_z^o is induced. The stress Φ_x^o is much lower than Φ_z^o since one expects $E/B_{/\!/} < 1$. In large samples there will be regions where the stress will exceed the critical stress Φ^c for nucleating dislocations. This will occur on parallel lines defined by z = const. One would have periodic emission of dislocations just as one has periodic emission of vortices in a Josephson junction. We shall not consider here the question of nucleation but rather a situation in which an isolated dislocation gets a uniform motion of velocity $\underset{\sim}{V}_o$ induced by the stress due the wedge (eqs. 19–22). The procedure is similar to the one defined in section 3. In fact the dynamical phase equation will differ from eq. 8, since Smectic C "Navier-Stokes" equations are different from Smectic A one. Strain field $\underset{\sim}{m}^d$ around dislocation and friction coefficients are given in ref. (3). Due to Smectic C symmetry properties, cross terms $\lambda_{xz} = \lambda_{zx}$ now exist in the expressions relating the applied stress $\underset{\sim}{\Phi}^o$ and the velocity $\underset{\sim}{V}_o$ of the dislocation :

$$P_z = -\varepsilon_d \Phi_x^o = \lambda_{xz} V_{ox} + \lambda_{zz} V_{oz} \tag{23}$$

$$P_x = \varepsilon_d \Phi_z^o = \lambda_{xx} V_{ox} + \lambda_{xz} V_{oz} \tag{24}$$

These relations imply both glide and climb motion of the dislocations.

$$V_{oz} = - \varepsilon_d(\lambda_{zz}\Phi_x^o + \lambda_{xz}\Phi_z^o)/(\lambda_{zz}\lambda_{xx} - \lambda_{xz}^2) \tag{25}$$

$$V_{ox} = + \varepsilon_d (\lambda_{zz} \Phi_z^o + \lambda_{xz} \Phi_x^o)/(\lambda_{zz} \lambda_{xx} - \lambda_{xz}^2) \tag{26}$$

where λ_{xz} is of the form $\lambda_{xz} = - E\lambda'$ and λ_{xx}, λ_{xy} and λ' are positive quantities. First let us notice that for a Smectic A analogy only climb motion is possible : $E = 0$ gives $\lambda_{xz} = \Phi_x^o = 0 \Rightarrow V_{oz} = 0$. One recovers the properties described in fig. 4. A change in the sense of rotation of the ellipse

$$E \rightarrow - E$$

implies : $\phi_z^o \rightarrow \Phi_z^o$

$$\phi_x^o \to -\phi_x^o$$

$$\lambda_{xx}, \lambda_{zz} \to \lambda_{xx}, \lambda_{zz}$$

$$\lambda_{xz} \to -\lambda_{zx}$$

which corresponds to :

$$V_{ox} \to V_{ox}$$

$$V_{oz} \to -V_{oz}$$

It is also clear from expressions 19-22 that a change $\theta \to -\theta$ affects neither Φ_x^o nor Φ_z^o in the central region, which corresponds to experimental observations. Let us now interpret the experimental observations : V_{oz} depends linearly on θ but $V_{ox} \sim$ const. For simplicity we consider the limit $E \ll B_{//}, B_{\perp}$ (This inequality is suggested by the fact that the strain pattern, as given by the Smectic A analogy provides a satisfactory account of experiments[2]) which gives :

$$V_{oz} \simeq -\varepsilon_d \, \Phi_x^o/\lambda_{zz}$$

$$V_{ox} \simeq \varepsilon_d \, \Phi_z^o/\lambda_{xx}$$

Since $\Phi_z^o \gg \Phi_x^o$ (ratio $B_{//}/E$) the critical stress Φ^c is first reached by Φ_z^o. Then Φ_z^o is bounded by Φ^c and one expects a velocity V_{ox} bounded by the critical stress. On the other hand, although Φ_x^o is much smaller than Φ_z^o, V_{oz} can be comparable or larger than V_{oz} since λ_{zz} is much smaller[3] than λ_{xx} (ratio $(B_{\perp}/B_{//})^2 \sim (0.06)^2$).

CONCLUSION

The natural question linked to the use of the analogy developed in this review is of course, how far can one goes without hitting a serious fundamental problem due to the profoundly different nature of far from equilibrium systems and thermodynamical one ? All the equations we have introduced are expected to hold in the so called hydrodynamic regime (i. e :long wavelength fluctuations and long time behavior). As such, they fail close to the core of the dislocations but do properly describe their far field pattern. This is a fairly standard statement for thermodynamical systems which holds in that case as well. For instance, the deformation pattern around a static edge dislocation calculated by de Gennes for Smectics, has been shown to be relevant to some cases of roll instabilities[14]. Taking account of dislocation motion and of more restricted symmetries, as we have shown here, allows to further exploit the analogies with thermodynamical systems. One can even say, that far from equilibrium roll structures allow to visualize phenomena which would be extremely hard to see directly in Smectics. For instance the very large asymmetry of the strain pattern of a moving dislocation can be seen by direct microscopic observation in the Nematic shear instability whereas it would require much more elaborate technics in Smectics. Similarly, the thermomechanical coupling, introduced by Leslie in Cholesterics[15], to interpret observations of Lehman at the beginning of the century has never been evidenced in Smectics : the continuous emission and motion of dislocations reveals the existence of its equivalence in far from equilibrium systems. Thus, with series of exemples in favour of the use of this analogy, one might think that it can be use without any precaution. There are however three fundamental differences between these classes of systems. First, the similarity of these equations results from the use of spatial symmetry and linearization ; in a system close to equilibrium one has additional symmetries due to time reversibility (Onsager reciprocal relation) which have no reason to hold in far from equilibrium systems. In fact, this is why there is no need to introduce an equation analogous to the heat transfer equation in the wedge problem. This absence of symmetry in the "transport" coefficient may have profond consequences. Secondly the far from equilibrium systems are essentially Brownian : to that respect they are simpler than Smectics for which a conventional hydrodynamic approach simply does not hold.[16] At last non linearities may be totally different in Smectics and roll systems.

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