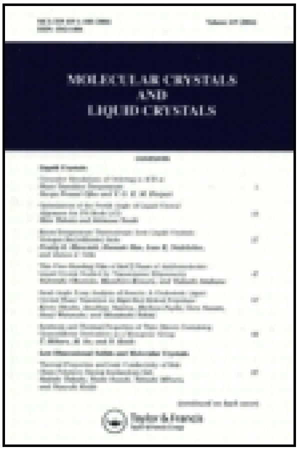

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Nemato-Dynamics of Two-Dimensional Defect Structures†

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A two-dimensional liquid crystal with a planar director field and perforated by a set of disclinations is studied for a given flow structure. The set of equations of motion governing the evolution of the director field and fluid flow is set up. This problem is mapped onto the collective state consisting of a set of disclinations and vortices moving in a potential flow. An effective Lagrangian for the disclinations and being equivalent to that used for 2 + 1-dimensional electrodynamics is tentatively proposed. Some aspects of the theory relative to the process of alignment of a liquid crystal under flow, and containing an intrinsic defect structure, are qualitatively discussed.

Keywords: liquid crystal polymers, phase transitions, shear flow

1. INTRODUCTION

If a polymeric melt or a liquid crystal is subject to shear or extensional flow, the phenomenon of shear thinning is observed. This is a consequence of the alignment of polymer molecules or of the director field of the nematic in the flow. For some liquid crystalline polymers[1] viscosity versus shear rate curves are observed as depicted in Figure 1, which has been reproduced from the work of Onogi and Asada,[2] and is commented by Asada in Reference 1 and by Marrucci.[3] This curve has a

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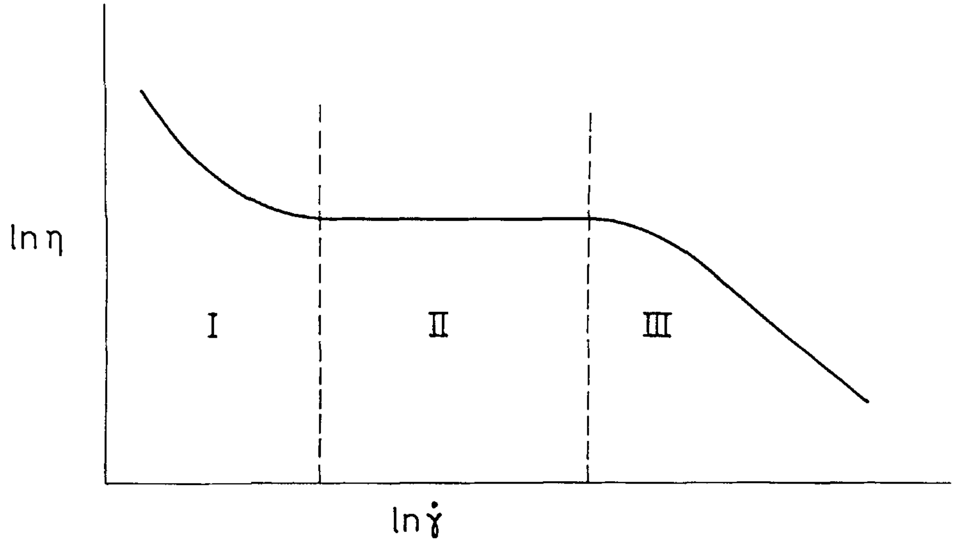

FIGURE 1 Schematic plot of the ln η vs. ln γ curve featuring the two shear thinning regimes I and III, and the Newtonian plateau II, according to Onogi and Asada.[2]

remarkable similarity with an isotherm in a p-V-diagram of a simple thermodynamic system undergoing a gas-liquid type phase transition, with the "Newtonian" plateau II in Figure 1 corresponding to the coexistence region. The shape of the curve $\ln\eta$ vs $\ln\dot{\gamma}$ in Figure 1 is certainly a function of the initial defect structure and the nature of the liquid crystal polymer. It is therefore suggestive that similar curves exist where domain II degenerates into an inflexion point, corresponding to the critical point of the p-V-diagramm, and then vanishes completely. Shear thinning has been studied by Yamazaki *et al.*[4] from a renormalization group point of view. If Figure 1 reflects a phase transition it occurs certainly far from equilibrium. In the following we will develop a theoretical basis of such a phenomena and study a number of related aspects connected with defect structures in two-dimensional nematics made up of disclinations and interacting with a hydrodynamic flow.

The plan of the paper is the following. In sect. 2 the basic formalism of nemato-dynamics is sketched. In sect. 3 an electromagnetic analogy applying to disclinations is indicated, and in sect. 4 the entropy production rate of a nematic defect structure in a nonuniform flow is studied. Conclusions are drawn in sect. 5.

2. BASIC FORMALISM

In the following the basic formulae of nemato dynamics as given e.g., by de Gennes[5] or Stephen and Straley[6] and specialized to the two-dimensional case will be briefly presented for a nematic with isotropic Frank's constants. Frank's energy is given by

$$\mathcal{F}' = \frac{1}{2} K \int d^2r(\nabla \mathbf{n})^2, \tag{1}$$

where $\mathbf{n} = (n_x, n_y)$ is a planar unit vector field imposed by suitable boundary conditions and K is Frank's constant for a specimen of thickness d.

The equation of motion for the angular velocity $\mathbf{\Omega}$ is

$$Jd\mathbf{\Omega}/dt = \mathbf{n} \times \mathbf{h} - \mathbf{\Gamma}, \tag{2}$$

where J is the moment of inertia per volume unit, and

$$\mathbf{\Omega} \equiv \mathbf{n} \times d\mathbf{n}/dt,$$

$$\mathbf{h} \equiv -\delta\mathcal{F}'/\delta\mathbf{n} = K\Delta\mathbf{n},$$

$$\Delta \equiv \partial^2/\partial x^2 + \partial^2/\partial y^2.$$

The frictional torque $\mathbf{\Gamma}$ is defined by

$$\mathbf{\Gamma} = \mathbf{n} \times \{\gamma_1\mathbf{N} + \gamma_2\mathbf{A}\cdot\mathbf{n}\}, \tag{3}$$

where

$$\mathbf{N} \equiv \frac{d\mathbf{n}}{dt} - \boldsymbol{\omega} \times \mathbf{n} = (\mathbf{\Omega} - \boldsymbol{\omega} \times \mathbf{n}, \tag{4}$$

$$\boldsymbol{\omega} \equiv \frac{1}{2}\nabla \times \mathbf{v}, \tag{5}$$

$$(\mathbf{A})_{ij} \equiv A_{ij} = \frac{1}{2}(\partial v_j/\partial x_i + \partial v_i/\partial x_j). \tag{6}$$

Here $\boldsymbol{\omega}$ and $\mathbf{A}$ represent vorticity and deformation rate of the fluid motion, respectively and $d/dt = \partial_t + (\mathbf{v}\cdot\nabla)$; γ_1 and γ_2 can be expressed through Leslie's coefficients $\{\alpha_i\}$ in the form $\gamma_1 = \alpha_3 - \alpha_2$, $\gamma_2 = \alpha_6 - \alpha_5$.

The acceleration equation of the fluid of mass density ρ is

$$\rho dv_i/dt = \partial\sigma_{ji}/\partial x_j, \tag{7}$$

where $\underset{\sim}{\sigma}$ is the stress tensor,

$$\sigma_{ij} = -p\delta_{ij} + \sigma^d_{ij} + \sigma'_{ij}. \tag{8}$$

Here the distorsion ($\boldsymbol{\sigma}^d$) and viscous ($\boldsymbol{\sigma}'$) stress tensor and the pressure p enter. They are defined by

$$\sigma_{ij}^d \equiv -\frac{\delta \mathcal{F}'}{\delta(\partial n_k/\partial x_i)}(\partial n_k/\partial x_j), \tag{9}$$

$$\sigma'_{ij} = \alpha_1 n_i n_j n_p n_q A_{pq} + \alpha_5 n_i n_p A_{pj} + \alpha_6 n_j n_p A_{pi} + \alpha_2 n_i N_j + \alpha_3 n_j N_i + \alpha_4 A_{ij}, \tag{10}$$

where the summation convention is used throughout, and incompressibility $\nabla \cdot \mathbf{v} = 0$, assumed; $\alpha_4/\rho = \nu$ represents the kinematic viscosity.

The entropy production rate due to fluid and director motion is

$$T\dot{S} = d\int d^2r[A_{ij}\sigma'_{ji} + \mathbf{f}' \cdot \mathbf{N}], \tag{11}$$

where the viscous torque is given by

$$\mathbf{f}' = (\alpha_3 - \alpha_2)\mathbf{N} + (\alpha_3 + \alpha_2)\mathbf{A} \cdot \mathbf{n}.$$

In the case that one ignores friction and the coupling between fluid motion and director field the set of Equations (2) and (7) reduces to

$$\left(\Delta - \left(\frac{J}{K}\right)\frac{\partial^2}{\partial t^2}\right)\Theta = 0, \tag{2'}$$

$$\rho\frac{d}{dt}\mathbf{v} = -\nabla p, \tag{7'}$$

where $\mathbf{n} \equiv (\cos\Theta, \sin\Theta)$, and $c = \sqrt{K/J}$ is the characteristic speed.

Soliton solutions of (2') and (7') are well known. Time-independent disclinations of (2') are described by[5]

$$\Theta^{(0)}(\mathbf{r},\{\mathbf{r}_i\}) = \frac{1}{2}\sum_i m_i \arctan\frac{y - y_i}{x - x_i}, \quad m_i = \pm 1, \pm 2, \ldots \tag{12}$$

and lead to a Frank energy

$$\mathcal{F}'_d = -\frac{\pi}{4}K\sum_{i\neq j} m_i m_j \ln\frac{|\mathbf{r}_i - \mathbf{r}_j|}{a} + \gamma\sum_i m_i^2, \tag{13}$$

where a and γ represent characteristic core radius and energy, respectively and the constraint

$$\sum_i m_i = 0 \tag{14}$$

has to be satisfied.

Vortex solutions of (7′) obey equations of motion derived from the Lagrangian[7]

$$L_\nu = \sum_i \omega_i(\dot{x}_i y_i - x_i \dot{y}_i) - \frac{1}{2}\sum_{i\neq j} \omega_i\omega_j g(\mathbf{r}_i, \mathbf{r}_j) - \frac{1}{2}\gamma_\nu(\mathbf{r}, \mathbf{r}) \sum_i \omega_i^2, \tag{15}$$

where

$$g(\mathbf{r}, \mathbf{r}') = -\frac{1}{2\pi} \ln \frac{|\mathbf{r} - \mathbf{r}'|}{a} + \gamma_\nu(\mathbf{r}, \mathbf{r}')$$

and $\gamma_\nu(\mathbf{r}, \mathbf{r}') = \gamma_\nu(\mathbf{r}', \mathbf{r})$ is a harmonic function used to satisfy special boundary conditions if needed. The set of vorticities is subject to the constraint

$$\sum_i \omega_i = 0. \tag{16}$$

The Lagrangian governing the time evolution of disclinations is obtained from

$$L_d = \frac{1}{2} K \int d^2r \left[\frac{1}{c^2}\left(\frac{\partial\Theta}{\partial t}\right)^2 - \left(\frac{\partial\Theta}{\partial x}\right)^2 - \left(\frac{\partial\Theta}{\partial y}\right)^2\right], \tag{17}$$

which leads to (2′) and into which one may plot $\Theta^{(0)}(\mathbf{r}, \{\mathbf{r}_i(t)\})$. Setting

$$L_d' = \varepsilon_{\mathrm{kin}}' - \mathcal{F}_d' \tag{17'}$$

one obtains

$$\begin{aligned}\varepsilon_{\mathrm{kin}}' = \frac{\pi}{8} J \sum_{i\neq j} \Bigg\{ & m_i\dot{x}_i m_j\dot{x}_j \left[\frac{1}{2}\cos 2\Phi_{ij} - \ln\frac{|\mathbf{r}_i - \mathbf{r}_j|}{a}\right] \\ & - m_i\dot{y}_i m_j\dot{y}_j \left[\frac{1}{2}\cos \Phi_{ij} + \ln\frac{|\mathbf{r}_i - \mathbf{r}_j|}{a}\right] + m_i\dot{x}_i m_j\dot{y}_j \sin 2\Phi_{ij}\Bigg\} \\ & + \gamma_k \sum_i (m_i\mathbf{v}_i)^2,\end{aligned} \tag{18}$$

where $2\gamma_k/J = \gamma/K$, $\Phi_{ij} = \arctan(y_i - y_j)/(x_i - x_j)$, $\mathbf{v}_i = (\dot{x}_i, \dot{y}_i)$, and the following constraints are imposed

$$\sum_i m_i = \sum_i m_i\mathbf{v}_i = 0. \tag{19}$$

They are necessary in order that L_d' does not diverge as log A where A is the area of the system. Observe that $\Theta^{(0)}$ ($\mathbf{r}$, $\{\mathbf{r}_i(t)\}$) does not satisfy (2′).

For non-vanishing friction and the approximation $d/dt \to \partial/\partial t$, (2) can be brought into the form

$$(\Delta - (\gamma_1/K)\partial_t - \frac{1}{c^2}\partial_t^2)\Theta = -(\gamma_1/K)\omega + (\gamma_1/K)[v_x\partial_x\Theta \sin^2\Theta + v_y\partial_y\Theta \cos^2\Theta] + (\gamma_2/K)[\sin 2\Theta A_{yy} + \cos 2\Theta A_{xy}], \quad (20)$$

where $\partial_\mu = (\partial/\partial t, \partial/\partial x, \partial/\partial y)$. The simplest approximation to (20), which may be treated exactly is

$$(\Delta - (\gamma_1/K)\partial_t - \frac{1}{c^2}\partial_t^2)\Theta = -(\gamma_1/K)\omega. \quad (20')$$

Observe that an improved version of (7′) takes coupling to the director field into account, i.e.,

$$\rho\frac{d}{dt}\mathbf{v} = -\nabla p + \nabla\cdot\boldsymbol{\sigma}^d$$

and yields

$$\rho\frac{d}{dt}\omega = \frac{1}{2}\nabla\times(\nabla\cdot\boldsymbol{\sigma}^d). \quad (21)$$

From this follows that in the presence of the nematic vorticity is not conserved.

3. ELECTROMAGNETIC ANALOGY

In the following an improved version of L_d' in the presence of friction and flow is derived. Normalizing time according to $ct \to t$, we obtain the action S_d corresponding to (17) in the form

$$S_d = \frac{1}{2}(JK)^{1/2}\int d^3x(\partial_\mu\Theta\partial^\mu\Theta), \quad (22)$$

where $(x^\mu) = (t, x, y)$, $\partial_\mu = \partial/\partial x^\mu$, $\partial_\mu\Theta\partial^\mu\Theta = \eta^{\mu\nu}\partial_\mu\Theta\partial_\nu\Theta$, and $\eta^{\mu\nu}$ is a Lorentz-metric for 2 + 1-dimensional space-time, whose non-vanishing diagonal is (1, −1, −1). Partial integration of (22) and use of (21) yields

$$S_d = \frac{1}{2}\gamma_1\int d^3x[\Theta\omega' - \Theta\partial_t\Theta] + \frac{1}{2}(JK)^{1/2}\int\Theta\partial_\mu\Theta[d^2a]^\mu, \quad (23)$$

where $\omega' \equiv (1/c)\omega$, and $[d^2a]^\mu$ represents the normal area element of oriented internal and external boundaries of the system. Internal boundaries[5] arise along the cuts originating from the cores of disclinations and give rise to the multivaluedness of Θ, see e.g., (12).

In order to integrate the second part of (23) we need to apply Stokes' theorem. Setting

$$\partial_\mu \Theta = (\text{rot } A)_\mu + \partial_\mu \Psi \tag{24}$$

where $A = (\Phi, \mathbf{A})$ is a 3-potential and rot A its rotation, $\partial^\mu(\text{rot } A)_\mu = 0$ implies that Ψ satisfies the equation

$$\left[\Delta - \frac{\gamma_1}{\sqrt{JK}}\,\partial_t - \partial_t^2\right]\Psi = -(\gamma_1/K)(\omega + cB), \tag{25}$$

where $B \equiv \partial_x A_y - \partial_y A_x$ represents the "magnetic induction" field. On the other hand rot $\partial\Psi = 0$ implies from (24) that A satisfies the equation

$$(\Delta - \partial_t^2)A = \begin{pmatrix} \partial_x\partial_y - \partial_y\partial_x \\ \partial_y\partial_t - \partial_t\partial_y \\ \partial_t\partial_x - \partial_x\partial_t \end{pmatrix}\Theta, \tag{26}$$

where Lorentz gauge $\partial_t\Phi + \partial_x A_x + \partial_y A_y = 0$ has been imposed. In the presence of singularities the rhs of (26) does not vanish. If singularities are parametrized by $\{\mathbf{r}_i(t)\}$ and are of the type contained in (12), (26) yields

$$(\Delta - \partial_t^2)A = \pi \sum_i m_i \delta^{(2)}(\mathbf{r} - \mathbf{r}_i(t))v_i, \tag{26'}$$

where $v_i = (1, \dot{x}_i, \dot{y}_i)$. Obviously the rhs of (26′) represents the 3-current density $-2\pi j^\mu = -2\pi(\rho, j)$, generated by the system of disclinations, and being conserved $\partial\rho/\partial t + \underset{\sim}{\nabla} \cdot \tilde{j} = 0$.

Integration of the second term of (23) for the first term on the rhs of (24) is now easily done, observing that Θ jumps along oriented internal boundaries by $-(\pi/2)m_i$, and applying Stokes' theorem. This yields

$$S_d^{(1)} = \frac{\pi}{2}(JK)^{1/2} \sum_i m_i \int_{C_i} [\mathbf{A} \cdot \mathbf{v}_i - \mathbf{\Phi}]dt \tag{27}$$

which is just the standard action of a system of moving charges interacting over their "electromagnetic" fields,[8] $\{C_i\}$ represents the set of space time trajectories of disclination cores, and $\Phi = \Phi(\mathbf{r}_i(t), t)$, etc. The first term in (27) represents the kinetic energy and the negative of the second term the potential energy.

The explicit form of $(\mathrm{rot}\, A)_\mu$ in (24) is

$$(\mathrm{rot}\, A)_\mu = (-B, E_y, -E_x), \tag{28a}$$

where

$$E_\mu = -\partial_t A_\mu - \partial_\mu \Phi, \quad \mu = x, y$$

yielding Faraday's law via

$$\partial^\mu (\mathrm{rot}\, A)_\mu = 0 = \partial_t B + \partial_x E_y - \partial_y E_x. \tag{28b}$$

Use of (26′) yields immediately Gauss' law

$$\nabla \cdot \mathbf{E} = 2\pi\rho. \tag{28c}$$

Observe now that (28) is invariant against the gauge transformation

$$\Phi \to \Phi' = \Phi - \partial_t \Lambda, \quad \mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\Lambda,$$

where Λ is a scalar function. This implies that we can use the radiation gauge, $\nabla \cdot \mathbf{A} = 0$. In that case (26′) is replaced by

$$\Delta\Phi = -2\pi\rho, \tag{29}$$

$$(\Delta - \partial_t^2)\mathbf{A} = -2\pi \mathbf{j}_t, \tag{30}$$

where $\mathbf{j}_t$ is the transverse current density, definded via

$$\mathbf{j} = \mathbf{j}_1 + \mathbf{j}_t, \quad \nabla \times \mathbf{j}_1 = \nabla \cdot \mathbf{j}_t = 0.$$

The action $S_d^{(1)}$ may be evaluated using (30) within the Darwin-approximation,[8] i.e., ignoring the ∂_t^2-term. This yields

$$L_d'' = -\frac{\pi J}{8} \sum_{i \neq j} m_i m_j \ln \frac{|\mathbf{r}_i - \mathbf{r}_j|}{a}$$

$$\left\{ \mathbf{v}_i \cdot \mathbf{v}_j + \frac{[(\mathbf{v}_i \cdot \mathbf{r}_{ij}^0)(\mathbf{v}_j \cdot \mathbf{r}_{ij}^0) - \mathbf{v}_i \cdot \mathbf{v}_j/2]}{2 \ln \dfrac{|\mathbf{r}_i - \mathbf{r}_j|}{a}} \right\}$$

$$+ \gamma \sum_i m_i^2 (1 - \sqrt{1 - v_i^2/c^2}) - \mathcal{F}_d'. \tag{31}$$

where $\mathbf{r}_{ij}^0 \equiv (\mathbf{r}_i - \mathbf{r}_j)/|\mathbf{r}_i - \mathbf{r}_j|$. The first and second term of (31) represent the kinetic energy stored in the director field and cores of disclinations respectively. L_d'' agrees with L_d' up to terms of order v_i^4/c^4, as a consequence of the instantaneous approximation used. The main difference between L_d and L_d' is that the second constraint in (19) is not needed for (31).

We consider next the contribution of the Ψ-field to the second term on the rhs of (23), denoted by $S_d^{(2)}$

$$S_d^{(2)} = \frac{\pi}{2}\sqrt{JK}\sum_i m_i \int_{D_i} \partial_\mu \Psi [d^2 a]^\mu, \tag{32}$$

where Ψ satisfies (25), and the space time domain D_i is bounded by C_i. The solution to (25) may be represented in the form

$$\Psi(x) = -\frac{1}{2\pi}\int d^3x' G_r(x, x')\zeta(x'), \tag{33}$$

where $\zeta(x) \equiv -(\gamma_1/K)(\omega + cB)$, $x \equiv (t, \mathbf{r})$ and $G_r(x, x')$ is the retarded Green's function[8] obeying

$$(\Delta - \frac{\gamma_1}{\sqrt{JK}}\partial_t - \partial_t^2)G_r(x, x') = -2\pi\delta^{(3)}(x - x').$$

Further analysis of (32) and (33) will be postpond to another publication. Here we state only the result for slowly moving disclinations yielding

$$S_d^{(2)} = -\pi^2\gamma_1 \sum_i m_i \int_{C_i} dt \int d^2r'(\omega(\mathbf{r}', t) + cB(\mathbf{r}', t))\arctan\left(\frac{y_i(t) - y'}{x_i(t) - x'}\right), \tag{34}$$

where the original time coordinate has been restored.

A certain problem with (34) is that its kernel is a multivalued function, and therefore is gauge dependent, i.e., it depends on the location of cut-lines associated with disclinations. This is a consequence of the fact that (32) and (34) have their origin in frictional processes and therefore count winding numbers. It is suggestive that the gauge dependence is compensated by the first term of (23), which can be computed from Θ, obtained as a path dependent function from (24).

A special case of interest is the limit $J \to 0$, or $c \to \infty$. In that case (26′) yields $\mathbf{A} = 0$, because for the $\mathbf{A}$-component its rhs carries a factor $1/c$ in original time t. However into (34) enters cB, and that implies that this quantity obeys the equation

$$\Delta c\mathbf{B} = \pi\nabla \times \sum_i m_i \delta^{(2)}(\mathbf{r} - \mathbf{r}_i(t))\mathbf{v}_i, \tag{35}$$

which is easily integrated with the Green's function $g(\mathbf{r}, \mathbf{r}') = -1/2\pi \ln|\mathbf{r} - \mathbf{r}'|/a$ and yields a finite contribution to (34). From this result follows, that a displacement of the core of a disclination by $\delta\mathbf{r}_i$ in the time interval Δt does not imply that the director field changes rigidly into $\Theta^{(0)}(\mathbf{r}, \{\mathbf{r}_i(t) + \delta\mathbf{r}_i\})$ but that its time-evolution is governed by the diffusion constant $D = \sqrt{K/\gamma_1}$.

4. ENTROPY PRODUCTION RATE AND FRICTIONAL FORCES

Consider first a set of moving disclinations in a fluid flowing at constant velocity $\mathbf{v}$. Entropy production according to (11) is given by

$$T\dot{S} = (\alpha_3 - \alpha_2)d \int d^2r[\partial_t\Theta + (\mathbf{v} \cdot \nabla)\Theta]^2, \tag{36}$$

where Θ obeys (20) with only the second term on the rhs of (20) nonvanishing. Evaluation of (36) using $\Theta^{(0)}(\mathbf{r}, \{\mathbf{r}_i(t)\}$ and $\mathbf{v} = (v_x, 0)$ yields

$$\begin{aligned} T\dot{S} = \frac{1}{4}(\alpha_3 - \alpha_2)d \Bigg\{ &\frac{8}{J}\varepsilon'_{\text{kin}} - \pi v_x^2 \sum_{i \neq j} m_i m_j \\ &\left[-\frac{1}{2}\cos\Phi_{ij} + \ln\frac{|\mathbf{r}_i - \mathbf{r}_j|}{a}\right] \\ &+ 4(\gamma/K)v_x^2 \sum_i m_i^2 + 2\pi v_x \sum_{i \neq j} \Bigg\{ m_i\dot{x}_i m_j \\ &\left[-\frac{1}{2}\cos\Phi_{ij} + \ln\frac{|\mathbf{r}_i - \mathbf{r}_j|}{a}\right] \\ &+ \frac{m_i\dot{y}_i m_j}{2}\sin 2\Phi_{ij}\Bigg\} - 8(\gamma/K)v_x \sum_i \dot{x}_i m_i^2 \Bigg\}, \end{aligned} \tag{36'}$$

where $\varepsilon'_{\text{kin}}$ and Φ_{ij} are defined by (18), and (19) applies. Equation (36′) allows the computation of frictional forces excerted by the fluid onto the disclinations via the formula

$$\mathbf{f}_i = -\frac{m_i}{2}\frac{\delta T\dot{S}}{\delta(m_i\mathbf{v}_i)} + \frac{m_i}{2}\frac{\delta T\dot{S}}{\delta(m_i\mathbf{v})}. \tag{37}$$

For $\mathbf{v} = \{\mathbf{v}_i)$ the frictional forces vanish due to $d\Theta^{(0)}/dt = 0$ and (36). Equation (36′) is a generalization of the formula given in Reference 6 for a single disclination at rest. Using the techniques of sect. 3, iteratively improved solutions to $\Theta^{(0)}(\mathbf{r}, \{\mathbf{r}_i(t)\})$ of (20) may be derived to evaluate (36).

A more interesting situation arises if the steady linear flow is considered[9]

$$\mathbf{v}(\mathbf{r}) = \mathbf{\Gamma} \cdot \mathbf{r}, \quad \mathbf{\Gamma} = \nu' \begin{Bmatrix} (1 + \lambda) - (1 - \lambda) \\ (1 - \lambda) - (1 + \lambda) \end{Bmatrix}, \tag{38}$$

where λ ranges in the interval $[-1, 1]$. This flow satisfies (7) for $\sigma^d \equiv 0$, has constant vorticity $\omega = \nu'(1 - \lambda)$ and $\nabla \cdot \mathbf{v} = 0$. For $\lambda = 1, 0, -1$ it represents pure extensional, shear and rotational flow, respectively. The linear stability properties of (7) for (38) and $\sigma^d \equiv 0$ have been studied by Lagnada et al.[10] It is found that all unbounded flows with $0 < \lambda \leq 1$ are unconditionally unstable.

A similar analysis of (7) in the presence of a nematic, can only be done in the aligned state, because otherwise disturbances are not infinitesimal. In that state the finite Frank elasticity of the nematic will stabilize the flow up to a critical velocity. A similar role is played by polymer elasticity in turbulent drag reduction (see e.g., Rabin and Zielinska[11]). In the presence of disclinations the rhs of (21) will not vanish and vortices will be generated by disclinations. In that case (38) should be replaced by a more general flow

$$\mathbf{v}(\mathbf{r}) = \mathbf{\Gamma} \cdot \mathbf{r} + \nabla \times (\Psi \hat{\mathbf{z}}), \tag{38'}$$

where Ψ is the stream function satisfying

$$\Delta \Psi = - \sum_{i=1}^{n} \omega_i \delta^{(2)}(\mathbf{r} - \mathbf{r}_i(t)).$$

Equation (20) approximately reads in that case

$$(\Delta - (\gamma_1/K)\partial_t - (1/c^2)\partial_t^2)\Theta = -\nu'(1 - \lambda)(\gamma_1/K) - (\gamma_1/K)\omega$$
$$+ (\nu'\gamma_1/K)\{[(x - y) + \lambda(x + y)]\partial_x\Theta \sin^2\Theta$$
$$+ [(x - y) - \lambda(x + y)]\partial_y\Theta \cos^2\Theta\}$$
$$- \nu'(1 + \lambda)(\gamma_2/K)\sin 2\Theta, \tag{39}$$

where ω is the vorticity due to the second term on the rhs of (38′).

Equation (39) features naturally three regimes, where the values of $\nu'(\gamma_i/K)_{i=1,2}$ are small compared to 1, of the order of 1, and large compared to 1, respectively. The regime (I) $\nu'(\gamma_i/K)_{i=1,2} \ll 1$ may be accessible by perturbation theory starting from $\Theta^{(0)}(\mathbf{r}, \{\mathbf{r}_i(t)\})$, or its improved version computed by the methods developed in sect. 3. The regime (III) $\nu'(\gamma_i/K)_{i=1,2} \gg 1$ carries a nematic structure, which is essentially determined by the operators on rhs of (39). There defects of disclination type may be rather scarce implying that $\omega \cong 0$, and the lhs of (39) may be treated by perturbation theory. The intermediate or crossover regime (II), where $\nu'(\gamma_i/K)_{i=1,2} \cong O(1)$ is certainly the most difficult to handle. It can be considered as the domain where the flow destroys successively the defect structure of the nematic. In regime I the defect structure is put under strain, and in regime II the elastic energy accumulated in the defect structure is released into the flow. Tentatively the three regimes may be identified with those of Figure 1.

For the sake of simplicity we study entropy production in regime I using $\Theta^{(0)}$ $(\mathbf{r}, \{\mathbf{r}_i(t)\}$ in (11) and ignore ω in (39). The leading contribution to $T\dot{S}$ will be

$$T\dot{S} \cong (\alpha_3 - \alpha_2)d \int d^2r\, N^2 + \text{const},$$

because all other terms involving trigonometric functions are bounded. The result is represented in the form

$$T\dot{S} \cong \frac{1}{4}(\alpha_3 - \alpha_2)d \left\{ \frac{8}{J}\varepsilon'_{\text{kin}} + \nu' \sum_{i,j} m_i \boldsymbol{\Psi}_{ij}^{(1)} \cdot \mathbf{v}_j m_j + \nu'^2 \sum_{i,j} m_i \Psi_{ij}^{(2)} m_j + 4\nu'^2(1-\lambda)^2 A \right\} + \text{const}, \tag{40}$$

where the constraints (19) and two additional constraints apply, arising from log A-terms. $\boldsymbol{\Psi}_{ij}^{(1)}$ and $\Psi_{ij}^{(2)}$ are functions of $\mathbf{r}_i$ and $\mathbf{r}_j$ and have dimension of length and length squared, respectively. In order to apply (37) to (40) one inverts (38) yielding

$$\begin{aligned} \mathbf{r} &= \frac{1}{4\lambda\nu'^2}\boldsymbol{\Gamma}\cdot\mathbf{v}(\mathbf{r}), \\ \partial/\partial v_i(\mathbf{r}) &= \frac{1}{4\lambda\nu'^2}\left(\Gamma_{1i}\frac{\partial}{\partial x} + \Gamma_{2i}\frac{\partial}{\partial y}\right), \quad i = x, y \end{aligned} \tag{41}$$

and applies (41) to (40).

An essential difference between the frictional force field derived from (36) and (40) is that due to the nonuniform velocity field (38), the field $\{\mathbf{f}_i\}$ derived from (40) is position dependent. Ericksen stress derived from (13) on the other hand will depend on coordinate differences. Accordingly one may conclude, that frictional forces and Ericksen stress acting on disclinations will not match up to zero, preventing stationary states of the type $\partial\mathbf{n}/\partial t = 0$.

The present approach may be generalized including a stochastic vorticity field as in (38′) for the calculation of $T\dot{S}$. In that case (40) will be replaced by a quadratic form involving the velocity fields of the driving flow (38), the disclinations and vortices.

How should one apply the formalism developed so far to a computation of the $\ln\eta$ versus $\ln\dot{\gamma}$ - curve depicted in Figure 1. In a stochastic approach, the expectation value of $T\dot{S}$ per defect (disclinations and vortices) may play the role of a local temperature. More precisely for dimensional reasons one may set

$$kT_{\text{eff}} \sim \langle T\dot{S}\rangle/(\nu'\langle N\rangle), \tag{42}$$

where $\langle N\rangle$ is the average number of defects. This average is defined with respect to the Boltzmann-Maxwell distribution featuring the statistical weight

$$\exp\{-[\varepsilon'_{\text{kin}} + \mathcal{F}'_d + \mathcal{F}_v + \mathcal{F}_i]/kT_{\text{eff}}\}, \tag{43}$$

where $\mathcal{F}_v$ is the vortex Hamiltonian obtained from (15) and $\mathcal{F}_i$ represents interaction terms. An estimate of the apparent viscosity may be obtained from

$$\langle T\dot{S}\rangle/(dAv'^2) \sim \eta_{\text{ap}}. \tag{44}$$

The details of the model have not been studied so far. In the simplest qualitative approach one may set

$$\langle T\dot{S}\rangle \sim (\alpha_3 - \alpha_2)v'^2 dAf_{\text{def}}(v', \lambda)$$

implying

$$\eta_{\text{ap}} \sim (\alpha_3 - \alpha_2)f_{\text{def}}(v', \lambda). \tag{45}$$

The quantity $f_{\text{def}}(v', \lambda)$ depends on the defect structure of the nematic flow. Its computation requires a suitable model for that defect structure and its evolution under flow. A renormalization group approach to this problem has been developed by Yamazaki et al.[4]

5. CONCLUSIONS

A formalism has been set up to treat defect structures of a two-dimensional nematic with a planar director field in a hydrodynamic flow. In sect. 3 it has been shown that disclinations in nematics in the presence of friction and vorticity can be handled by methods familiar from electromagnetism. Physical quantities like the apparent viscosity η_{ap} of a nematic containing an intrinsic defect structure and being subject to a nonuniform but steady flow, are suggested to be computed by means of a stochastic formalism as indicated in sect. 4. The problem of evolution of a defect structure under flow condition has not been tackled. Physically it requires that the defect structure consisting of an intricate network of disclinations in a quasi-two-dimensional geometry is disentangled by the flow. This is achieved by pulling the set of defects through a hierarchy of potential barriers. The small barriers are overcome in the initial part of regime I in Figure 1, and the highest barriers reside at its end, whereas in regime II the nematic supposedly is cleared out of its defect structure. It is the stochastic nature of this process, and the transition of bound states of disclinations in regime I, into unbound states in regime II, which reminds of the Kosterlitz-Thouless[12] transition and is at the basis of the speculation that Figure 1 reflects a phase transition.

The formalism presented may be extended to three-dimensional nematics in a two-dimensional flow geometry. Extending the formalism to two-dimensional director fields is more difficult, although possible using the formalism developed in Reference 13 for the O(3)-σ-model. A more serious problem is posed by the extension to liquid crystal polymers requiring anisotropic Frank couplings, and differences in the mobility of disclinations of opposite strength. The dynamics of disclinations in such systems has been studied by Rieger[14] rather successfully using stochastic methods.

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