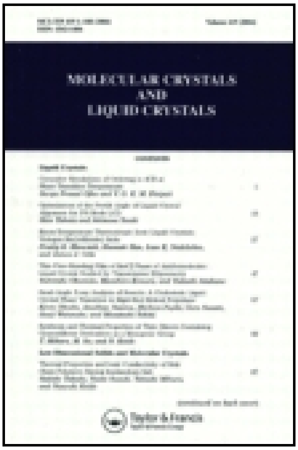

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The Hydrodynamics of Disclinations in Nematics

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The Hydrodynamics of Disclinations in Nematics*

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A theory of nematohydrodynamics in the presence of a small amount of disclinations is given. The Ericksen-Leslie theory is contained within it. Scaling found by Ericksen in normal nematohydrodynamics is not a property of the new theory. However for Poiseuille flow in a capillary, it is shown that disclinations lying along the flow are consistent with the equations; moreover, for such a case there is effectively Ericksen scaling, and consequently universal dependences previously predicted for effective viscosities should hold.

INTRODUCTION

The full Ericksen-Leslie equations (see *e.g.* Leslie)[1] for hydrodynamic motion in nematics has had success in a fully nonlinear analysis of simple flow situations. Flow alignment in Poiseuille flow for homogeneous alignment in nematics with viscosity α_3 negative is one example. In addition to specific analyses of flow, Ericksen noticed an invariance of the equations under a scaling of the spatial and time coordinates.[1] If the spatial coordinate was scaled by a factor, it was necessary to scale the time coordinate by the square of the same factor; the director remains unchanged by such a transformation. This gives a universal law for the effective viscosity in terms of flow rates and dimensions of flow channels which is quite distinct from that for isotropic viscoelastic fluids (Fisher and Fredrickson).[2] However, it is difficult to control the disclinations (de Gennes),[3] both line and point, which tend to occur in liquid crystal materials, and it may be that these

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disclinations are responsible for some of the anomalous results of Fisher and Fredrickson.[2] It is of interest to describe the effect of these defects in the hydrodynamics of nematics. There is a large number of disclination types, and it does not seem practical to have terms in the equations for each of them. Further, it is not clear that in the hydrodynamic regime of flow characterized by small wave vectors and frequencies all defects are relevant (Sarkar).[4] An aid to the analysis of such questions has been homotopy theory introduced by Toulouse and Kléman[5] in the study of condensed matter systems. It was found that topologically stable line defect strengths are additive modulo two (Dzyaloshinskii)[6], i.e., two lines of unit strength annihilate each other. This is unlike the situation for crystal dislocations, where the additive nature of dislocations allows the introduction of dislocation density and dislocation currents. It is not possible to follow a similar analysis for disclinations in nematics. Dzyaloshinskii and Volovik[7] have proposed a so-called Yang-Mills vector potential to describe the disclinations. It is easy to see why such an entity is relevant to study disclinations, but it is harder to understand its relevance in the construction of a suitable hydrodynamics. At a disclination line or point, a director is singular and also its derivative is not defined. If a director is defined by a rotation R from a reference direction, then $R\partial/\partial X_i R^{-1}$ is an object which transforms as a Yang-Mills field (Dzyaloshiniskii);[6] when the ith spatial derivative of R^{-1} does not exist it is convenient to introduce a quantity A_i which transforms as $R\partial/\partial X_i R^{-1}$ under rotations, i.e. like a Yang-Mills field representative of the SO(3) group.

Dzyaloshiniskii and Volovik[7] consider the situation when there is a dense mass of disclinations, and consequently the concept of director is not applicable. They proceed to formulate a hydrodynamics whose consequences are not known; also the explicit nature of friction laws (a crucial contribution of Leslie in the Ericksen-Leslie theory) was not discussed by them. As pointed out by us[4] it is possible that the disclinations will screen each other and there will be no long-range correlations between disclinations. Since no conservation laws are associated with disclinations and there are no long-range correlations in the susceptibility (at zero frequency), usual formulations of hydrodynamics[8] will exclude such variables from appearing in the hydrodynamics. We may well expect the disclinations to give an effective isotropic fluid with viscosity coefficients renormalized from those found in the isotropic phase of the nematics. The attractive aspect of this conclusion is that it agrees with intuition. In order to be able to make direct comparisons with experiments, it is necessary to be able to treat theoretically situations in which disclinations are localized and the director is defined outside some limited regions.

In this paper we will formulate a candidate for such a theory. In the limit of no disclinations, the Ericksen-Leslie theory emerges. Poiseuille flow in a capillary with homeotropic alignment is analyzed. It is found that disclination lines align with the flow in this particular geometry. The disclinations do not affect the scaling arguments of Ericksen. However, the full equations themselves do not admit an invariance of the scaling type proposed by Ericksen. It is just possible that the (admittedly limited) data for parallel alignment Poiseuille flow given by Fisher and Fredrickson[2] is incompatible with the predictions of Ericksen-Leslie theory owing to the presence of disclinations in the samples.

Following Dzyaloshinskii,[6] it is possible to write the matrix valued differential form RdR^{-1} as $\sum A^a l^a$ where l^a (a = 1, 2, 3) are the generators of SO(3). In terms of Euler angles (with the conventions used by Goldstein[9]) we have

$$\begin{aligned} A^1 &= -\sin\psi d\theta \qquad -\sin\theta\cos\psi d\phi \\ A^2 &= \cos\psi d\theta \qquad -\sin\theta\sin\psi d\phi \\ A^3 &= d\psi + \cos\theta d\phi \end{aligned}$$

When disclinations are present, the angles θ, ϕ, and ψ are not single valued and so the associated differential forms are not exact.[6] In addition, the director vector is invariant under changes in ψ. This gives rise to a gauge invariance. The director configuration is invariant when

$$A^3 \to A^3 + d\chi \tag{2}$$

where χ is a single valued function. The combinations $A^1 \pm iA^2$ are transformed by multiplicative factors $e^{\pm i\chi}$, and so are not gauge variables with respect to this transformation. From the expectation that a gauge variable has long range correlations, A^3 (to be denoted from now on by A) will be regarded as a hydrodynamic variable whereas $(A^1 \pm iA^2)$ will not be hydrodynamic variables. This is an economic choice and will be shown to be satisfactory for a simple and relevant situation. A planar configuration will be considered in coordinates such that in cartesian coordinates we have

$$\mathbf{n} = (\cos\phi, \quad \sin\phi, \quad 0) \tag{3}$$

and the reference vector $\mathbf{n}_0$ say will be chosen to be (1, 0, 0). The resulting rotation vector R is given by

$$R = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{4}$$

In a particular choice of gauge

$$A = \mathrm{d}\phi \tag{5}$$

If there is a disclination situated at $\mathbf{x}_0$ in the $z = 0$ plane, then it is necessary that

$$(\nabla \times \mathbf{A})_3 = 2\pi\delta(\mathbf{x} - \mathbf{x}_0) \tag{6}$$

This is a satisfactory description of the disclination line. For the hydrodynamic variables we will take $\mathbf{v}$, the velocity, $\mathbf{n}$, $\mathbf{A}$ and the pressure p. For simplicity, incompressible fluids will be considered. Near the disclination singularities, the director and its derivatives will be taken to approach zero; the singular structure is adequately described by the A variable.

The derivation of hydrodynamic equations will proceed as outlined by de Gennes[3] who, in turn, was influenced by de Groot and Mazur.[10] For an isothermal process, the dissipation is given as the sum of the rate of change of the total kinetic energy and the Frank free energy, the free energy of the disclinations, internal free energy, and a magnetic free energy. The magnetic free energy is taken to have the same form as in conventional theory. The free energy of the disclinations themselves is a scalar, and gauge invariant, and the simplest form of this is the integral over all space of the square of curl A. Furthermore in the constitutive equations we will not permit spatial derivatives of A except in expressions for molecular fields. This is similar in spirit to ignoring spatial derivatives of the director in constitutive equations by Leslie. Moreover, as usual, a linear relation between fluxes and conjugate forces is assumed.[10]

The resulting equations are the following:

$$\rho\frac{\mathrm{d}}{\mathrm{d}t}v_\beta = \partial_\alpha(\sigma^{\varepsilon}_{\alpha\beta} + \sigma'_{\alpha\beta}) \tag{7}$$

where

$$\begin{aligned}\sigma^{\varepsilon}_{\alpha\beta} = p\delta_{\alpha\beta} &+ 2g(\partial_q A_\alpha - \partial_\alpha A_q)(\partial_\beta A_q - \partial_q A_\beta)\\ &- (K_1(\nabla\cdot\mathbf{n})\delta_{\alpha\gamma} + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n})\varepsilon_{\alpha\gamma_i n_i}\\ &+ K_3(\mathbf{n}\cdot\nabla n_\gamma)n_\alpha)\partial_\beta n_\gamma\end{aligned} \tag{8}$$

and

$$\begin{aligned}\sigma'_{\alpha\beta} = \alpha_1 n_\alpha n_\beta n_\mu n_\rho e_{\mu\rho} &+ \alpha_4 e_{\alpha\beta} + \frac{1}{2}n_\alpha n_\mu e_{\mu\beta}(\alpha_5 + \alpha_6 - \gamma_2')\\ &+ \frac{1}{2}n_\beta n_\mu e_{\mu\alpha}(\alpha_5 + \alpha_6 + \gamma_2') + \frac{1}{2}(\gamma_2 - \gamma_1)n_\alpha N_\beta\\ &+ \frac{1}{2}(\gamma_2 + \gamma_1)n_\beta N_\alpha\end{aligned} \tag{9}$$

and

$$\mathbf{N} = \dot{\mathbf{n}} - \boldsymbol{\omega} \times \mathbf{n} \tag{10}$$

and

$$\boldsymbol{\omega} = \frac{1}{2}(\nabla \times \mathbf{v}) \tag{11}$$

and

$$e_{\alpha\beta} = \frac{1}{2}(\partial_\alpha v_\beta + \partial_\beta v_\alpha) \tag{12}$$

Furthermore

$$h_\mu = \gamma_2' n_\alpha e_{\alpha\mu} + \gamma_1 N_\mu \tag{13}$$

where h_μ the molecular field has the following expression

$$\begin{aligned} h_\mu = K_1\partial_\mu(\nabla \cdot \mathbf{n}) + K_2\partial_\gamma[(\mathbf{n} \cdot \nabla \times \mathbf{n})\varepsilon_{\gamma\mu i}n_i] + K_3\partial_\gamma((\mathbf{n} \cdot \nabla n_\mu)n_\gamma) \\ -K_2(\varepsilon_{pqr}n_p\partial_q n_r)(\varepsilon_{\mu jk}\partial_j n_k) - K_3(n_l\partial_l n_i)\partial_\mu n_i \\ + \gamma_a(\mathbf{n} \cdot \mathbf{H})H_\mu \end{aligned} \tag{14}$$

All the symbols not defined have standard meanings[3] and

$$j_\mu = \gamma_3 n_\mu n_\alpha \mathring{A}_\alpha \tag{15}$$

where

$$j_\mu = -2g\partial_\alpha(\partial_\mu A_\alpha - \partial_\alpha A_\mu) \tag{16}$$

and g is a material parameter associated with disclinations and γ_3 is a viscosity associated with the disclinations. These equations are supplemented with the divergence-free condition of the velocity field (necessary for incompressible flow). When A is zero, the equations reduce to those of Ericksen-Leslie.

It is convenient to consider Poiseuille flow in a capillary with homeotropic alignment, since in other flows a complex nonlinear regime precedes the appearance of disclinations. In cylindrical coordinates the following ansatz is made

$$\begin{aligned} &v_\rho = v_\phi = 0 \\ &v_z = u(\rho) \\ &n_\rho = \cos\psi(\rho)\sin\theta(\rho), \qquad n_\phi = 0, \qquad n_z = \cos\psi(\rho)\cos\theta(\rho) \\ &A_\phi = C(\rho), \qquad A_\rho = A_z = 0 \end{aligned} \tag{17}$$

The disclination terms appear explicitly in Eqs. (8), (15) and (16). From the ansatz (17) it is seen that

$$C''(\rho) + \frac{1}{\rho}C'(\rho) - \rho^{-2}C(\rho) = 0$$

which has a solution

$$C(\rho) = \alpha\rho^{-1} + \beta\rho$$

where α and β are constants. Owing to the form of the γ_3 term in Eq. (15), any slight time dependence cannot destabilize the solution. Curl **A** is in the z-direction and of magnitude 2β. The direction of curl **A** is the direction of disclination lines contributing to curl **A**; so the disclination lines are parallel to the flow.

Moreover the divergence of the disclination term in $\sigma^e_{\alpha\beta}$ vanishes for this solution. Hence, the equations for **v**, **n** and p are effectively decoupled from the disclinations in this geometry, and it should not then be surprising that Ericksen scaling holds in this geometry. The equations as a whole however are not invariant under scaling. The scaling property of A is taken to be that of RdR^{-1} and so we have

$$A^* = \lambda A$$

when

$$\mathbf{x}^* = \lambda^{-1}x$$

and λ is a scaling factor.

The asterisk denotes the scaled variable. In the expression for $\sigma^e_{\alpha\beta}$, the term $(\partial_q A_\alpha - \partial_\alpha A_q)(\partial_\beta A_q - \partial_q A_\beta)$ has different scaling properties from $(\nabla \cdot \mathbf{n})\partial_\beta n_\alpha$, since **n** is invariant under scaling according to Ericksen (Leslie).[1] We can hence conclude that the equations as a whole do not have a scaling invariance.

CONCLUSIONS

A model for treating hydrodynamics of disclinations in nematics has been presented and the consequences analyzed for Poiseuille flow. The conclusions so far are consistent with experiment. It is also suggested that nonuniversal (nonscaling) behavior found by Fisher and Fredrickson[2] in some experiments may possibly be due to disclinations which in the above model can cause scaling to break down for general configurations; at the same time scaling can be preserved for specially symmetric configurations.

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