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Invariant integrals applied to nematic liquid crystals with small Ericksen number and topological defects

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ABSTRACT

Invariant integrals are derived for nematic liquid crystals and applied to materials with small Ericksen number and topological defects. The nematic material is confined between two infinite plates located at $y = -h$ and $y = h$ ($h \in \Re^+$) with a semi-infinite plate at $y = 0$ and $x < 0$. Planar and homeotropic strong anchoring boundary conditions to the director field are assumed at these two infinite and semi-infinite plates, respectively. Thus, a line disclination appears in the system which coincides with the z-axis. Analytical solutions to the director field in the neighbourhood of the singularity are obtained. However, these solutions depend on an arbitrary parameter. The nematic elastic force is thus evaluated from an invariant integral of the energy–momentum tensor around a closed surface which does not contain the singularity. This allows one to determine this parameter which is a function of the nematic cell thickness and the strength of the disclination. Analytical solutions are also deduced for the director field in the whole region using the conformal mapping method.

1. Introduction

The hydrodynamic behaviour of a uniaxial nematic liquid crystal depends on both a velocity vector field $\mathbf{v}$ and a unit director vector field $\mathbf{n}$ with the spatial orientation defined by the twist and tilt angles. The director field is also considered to be non-polar such that the states $\mathbf{n}$ and $-\mathbf{n}$ are indistinguishable. The velocity field is constrained by the incompressibility condition $v_{i,i} = 0$ and the director field by $n_i n_i = 1$ $(i = 1, 2, 3)$ (see, e.g., Stewart (2004) and Atkinson and Pereira (2005a)).

In this work, invariant integrals for nematic liquid crystals are derived and applied to uniaxial materials with topological defects. Here, we consider model flow regimes with small Ericksen number. This means that we can neglect the response of the director to the flow field and just use the static director field for $\mathbf{v} = \mathbf{0}$ (see Atkinson and Pereira (2005b, 2006)). We obtain the energy–momentum tensors for uniaxial materials in Cartesian coordinates. We show that these second order rank tensors are spatially invariant using the angular momentum equations in flow regimes with small Ericksen number and no external body forces. As a consequence, the nematic elastic force is given by a closed surface integral of the energy–momentum tensor. Thus, one can prove that this closed surface integral is invariant using the divergence theorem.

It is well known that point singularities, line disclinations or surface defects appear in certain materials and can be induced by external forces like electric, magnetic or electromagnetic fields as well as by rubbing or cleaning the plate surfaces

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with an appropriate acid or detergent. Thus, one can obtain specific orientations for the director field at the plate surfaces (see de Gennes and Prost (1993) or Jenkins and Barratt (1974)). Here, we consider a uniaxial nematic liquid crystal confined between two infinite plates located at $y = -h$ and $y = h$ ($h \in \Re^+$) with a semi-infinite plate at $y = 0$ and $x < 0$. Planar and homeotropic strong anchoring boundary conditions to the director field are assumed at these two infinite and semi-infinite plates, respectively.

We assume the strong anchoring boundary conditions to the director field here to proceed with a specific application of the invariant integrals. It is well known that polishing the surfaces perfectly to obtain a definite orientation of the director field is not possible in practise, i.e., these boundary conditions cannot be achieved in practise. For any given situation our invariants will still apply though the subsequent calculation might not be so simple. An alternative and more recent mathematical approach to modelling anisotropic fluids has been suggested by Rajagopal and Srinivasa (2001) in which they assert that the specification of boundary conditions to the director field are not required since its approach is not a director theory. This may avoid any criticism with respect to perfect polishing. In fact, the mathematical approach proposed by Rajagopal and Srinivasa (2001) does not require specifying any additional boundary conditions other than that usually specified for viscous fluids, even for flows that involve spatially inhomogeneous fields.

However, with any theory there is always the pragmatic test of comparison with experiment and although no specific comparison is made in the present paper this will always be an issue as more detailed observation and interpretation of experimental results become available. This may even apply to the possibility of surface preparation which will improve as the technology advances. With these reservations, we proceed with the strong anchoring boundary conditions to the director field.

Thus, a 1/2 line disclination appears in the system which coincides with the z-axis. It is well known that disclinations of half-integer charge do not benefit from escaping into the third direction. We stress that according to Frank's definition the topological charge of a line defect is defined as the number of turns the director performs along a closed path surrounding the defect. Thus, we restrict the study to the situation in which the director field lies on the xoy plane. This means that a point defect is considered at the origin of the xoy Cartesian coordinate system.

Analytical solutions to the director field are deduced using the angular momentum equations for flow regimes with small Ericksen number and no external body forces. As the order of magnitude of the nematic elastic coefficients is nearly the same, the one elastic constant approximation for the elastic free energy density is considered in this work. However, these solutions which are valid in the neighbourhood of the singularity depend on an arbitrary parameter. Thus, the nematic elastic force is evaluated from an invariant integral of the energy–momentum tensor around a closed surface which does not contain the singularity. This singularity has a half-integer charge of 1/2. This allows one to determine this parameter which is a function of the disclination strength $m = 1/2$ and the nematic cell thickness $2h$. Exact solutions are also derived for the director field in the whole nematic region using the conformal mapping method. Moreover, we emphasise that regions with a lower free energy density grow at the expense of regions with a higher free energy density. This happens here due to the imposed strong anchoring boundary conditions to the director field at the two infinite and semi-infinite plates. Thus, assuming flow regimes with small Ericksen number and a steady state motion, the semi-infinite plate and the line disclination can be considered as moving together with a constant and positive velocity v in the opposite direction of the x-axis. This constant velocity depends on the core radius and the thickness of the nematic cell. The velocity of the line disclination as well as of the semi-infinite plate is estimated from the balance between the loss in free energy and the energy dissipated during the motion.

The plan of this paper is as follows. We begin with the Ericksen–Leslie partial differential equations in Cartesian coordinates for uniaxial nematic liquid crystals (see Section 2). In Section 3, the energy–momentum tensors are deduced for materials with small Ericksen number and no external body forces in Cartesian and cylindrical polar coordinates. The finite width strip problem is formulated and analytical solutions of the angular momentum equations to the nematic director vector field in the neighbourhood of the singularity are also investigated here. Furthermore, a relationship given by an invariant integral is deduced. The force exerted over a closed surface surrounding the nematic region is thus defined. The arbitrary parameter involved in the director solutions is calculated and a physical interpretation is given. The director vector field in the neighbourhood of the disclination with a half-integer charge of 1/2 is thus determined. Moreover, exact solutions are also derived in the whole strip using the conformal mapping method. Note that for the example shown (i.e., the one elastic constant approximation), we could have derived an invariant for the particular equations of the problem (see, e.g., (3.38)). However, this just serves as a check on the general method which should work for much more complicated energy functions of the nematic including the many elastic constant approximation. The constant velocity of the line disclination as well as of the semi-infinite plate is also estimated here. Finally, it is shown in Appendix A that the director correction term due to the nematic flow is of the order of the Ericksen number.

2. Governing partial differential equations

The equations describing the hydrodynamic behaviour of a uniaxial nematic liquid crystal are well known (see Ericksen (1961); Leslie (1968); Stewart (2004)). For completeness, these equations are presented here in Cartesian coordinates. The flow of a nematic liquid crystal is described by the velocity vector field $\mathbf{v}$ together with a director field $\mathbf{n}$, which is considered in this work as a non-polar unit vector giving the orientation of the anisotropic axis in these transversely isotropic liquids. With the assumption of incompressibility, the equations are the constraints