Nematodynamics on the basis of Landau-de Gennes Tensorial Approach

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Abstract In this paper we shall examine the nematodynamics which involves both the microscopic order parameters and the macroscopic director based on Landau-de Gennes theory of nematics. Introducing Lagrange multipliers corresponding to the conservation of trace of the tensor order parameter, the threshold condition of planar alignment cell will be first analytically derived to show the agreement with the conventional vector approach on the basis of Oseen-Zocher-Frank theory. In addition some practical numerical computational results will be presented so as to describe the relationship between the microscopic orders and the macroscopic director alignments under a certain external field. In practice, the microscopic orders are found to be affected by the external field as well as the anchoring strength at the boundaries.

Keywords: nematodynamics, elastic theory, Landau-de Gennes, Oseen-Zocher-Frank

§1. Introduction

Up to date, the elastic properties of nematics have been clarified extensively based on the continuum framework originated from Oseen-Zocher-Frank[1-3] theory with the director $n_{ij}$ such that $n_{ij}n_{ji}=1$ and on the Landau-de Gennes phenomenological theory with the tensor order parameter $Q_{ij}$ such that $\text{Tr}(Q)=0$ and $Q_{ij}=Q_{ji}$.[4,5]. The former vector approach has been involved in the hydrodynamic theory of nematics which is well known as Ericksen-Leslie theory[6,7]. On the other hand, the latter tensorial approach has been formulated to involve the hydrodynamics later[4,8]. In principle, however, these two approaches have to be related to each other in terms of the following explicit expression for the tensor order parameter

$$Q_{ij}=\frac{3}{2}\left(\frac{1}{3}\delta_{ij}+b_{ij}\right)+\frac{1}{2}\left(b_{ij}c_{ie},c_{ej}\right),$$

where $S$ and $A$ are the microscopic order parameters related to the uniaxial and biaxial orderings of molecules[9], respectively, the orthonormal triad vector set $a_i \cdot b \cdot c$ with $a = n$ is assumed to be the right-handed triad set hereafter. Recently the present author reported a general expansion of the elastic free energy expressions of the biaxial cholesterics[10] and the biaxial smectics[11] in terms of

$$F = \sum_{ijkl} K_{ijklmn} (a_i \cdot b \cdot c \cdot d) Q_{ijkl} Q_{mnop} + \sum_D q_{ij} (a_i \cdot b \cdot c \cdot d) Q_{ij},$$

where $K_{ijklmn}$ and $D_{ijkl}$ are the tensorial coefficients, which are to be determined to satisfy symmetry of the system and to be related to the orthonormal triad basis, or $a_i \cdot b \cdot c$, which also implicitly involves $\delta_{ij}$ and $\epsilon_{ijk}$ there[10-13].

In this work let us mention the nematodynamics within the tensorial form and apply it to the dynamics under an external field. In §2 theoretical framework will be mentioned in brief. Then §3 and §4 are devoted to some numerical results and conclusions, respectively.

§2 Theory

In this section we shall show the relationship between the tensorial and vector approaches restricting ourselves to the time-dependent Ginzburg-Landau (TDGL) approach. Hereafter let us focus our interest on the uniaxial nematics which may be characterized by somewhat modified tensor order parameter without any loss of generality.[14]

$$q_{ij}=n_i \cdot n_j = S a_{ji} \times (a_i \cdot n \cdot n) \quad (a_i \cdot n \cdot n),$$

where $S$ is the microscopic order parameter related to the molecular ordering along the director, $n$. The total free energy can be expressed as in the following form in terms of the tensor order parameter $q_{ij}$.

$$F(q_{ij},q_{ijk}) = \frac{L}{2} q_{ij} q_{ij} + 2L q_{ijk} q_{ijk} + \frac{1}{2} \epsilon_{ijk} q_{ijk} q_{ijk} + \frac{1}{2} A q_{ij} q_{ij} + B q_{ijk} q_{ijk} + C q_{ij} q_{ij} + q_{ij} q_{ij}$$

$$= F(q_{ij},q_{ijk}) + F(q_{ij},q_{ijk}) + F(q_{ij},q_{ijk}) + F(q_{ij},q_{ijk});$$

here we defined the following free energy components

$$F(q_{ij},q_{ijk}) = \frac{L}{2} q_{ij} q_{ij} + 2L q_{ijk} q_{ijk} + \frac{1}{2} \epsilon_{ijk} q_{ijk} q_{ijk},$$

$$F(q_{ij},q_{ijk}) = \frac{1}{2} \epsilon_{ijk} q_{ijk} q_{ijk},$$

$$F(q_{ij},q_{ijk}) = \frac{A}{2} \text{Tr}(q_{ij}^2),$$

$$F(q_{ij},q_{ijk}) = \frac{B}{3} \text{Tr}(q_{ijk}^2),$$

$$F(q_{ij},q_{ijk}) = \frac{C}{4} \text{Tr}(q_{ikj}^2).$$

In the above notations, $L$ and $q$ are the elastic constant and the chirality, respectively, $\epsilon_{ijk}$ the dielectric (or magnetic) anisotropy with $S=1$, $E_\perp$ the external electric (or magnetic) field, and $A, B, C$ are the phenomenological constants related to isothermal component $F_0(S)$ which may involve the nematic-isotropic phase transitions.
§3. Numerical Results

In this section, we shall focus on the non-chiral nematics in the planar cell under the external filed and examine the dynamics numerically. Thus our result can be described in terms of

$$q_{ij} = S_{ij} n_z, \; \; n_1, n_2, 0 = \begin{bmatrix} q_{11} & q_{12} & 0 \\ q_{21} & q_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix} n \cdot (n_1, n_2, 0),$$

(8)

$$q^* = 0 \; \; \text{(non-Chiral)}$$

$$e_{ij} = S_{ij} (\text{external field along } n_z)$$

Thus eq.(20) may be reduced to

$$\frac{\partial q}{\partial \tau} + \frac{\partial^2 q}{\partial \eta^2} = \pi^2 e_{ij} c (S \cdot S) q_{ij} + q \cdot \delta_{ij} + (\mu * q) \cdot \mu.$$  (10)

In Fig.1, we shall present an example of the nematodynamics under the conditions such that \( e=5, \; c=10^{-3}, \; S_0=0.8, \; S_1=0.6, \; S(0)=S(1)=1. \)

![Nematic Dynamics Example](image)

(a) Initial Condition of \( q(y) \)

(b) Final State of \( q(y) \)

Fig.1 An example of the numerical result for eq.(23) with \( e=5, \; c=10^{-3}, \; S_0=0.8, \; S_1=0.6, \; S(0)=S(1)=1 \) for a homogeneous planar cell with \( \theta(0)=\theta(1)=0.01. \)

§4. Conclusions

In this paper we have proposed a general expression of TDGL equation of nematodynamics in a tensorial form taking certain Lagrange multipliers into account. It has been found that the Lagrange multipliers are required to support the relation between the tensorial approach and the vector one. In addition we have presented an explicit tensororial expression for the Frank elastic free energy with three independent elastic constants based on the general second-order expansion in terms of \( Q_{ijk} \) as defined by eq.(2). Therefore it should be noted that such degeneracy between the splay and the bend elastic constants as presented in the previous works[4,5] can be removed within the generalized second-order expansion of \( a_{ijk} \) or \( Q_{ijk} \) including the orthogonal basis \( a-b-c \) into the tensorial expansion coefficients \( K_{ijk}(a \cdot b \cdot c) \) and \( D_{ijk}(a \cdot b \cdot c) \) as similar manner in the previous works related to the biaxial cholesterics and smectics[10-13]. In such an approach, all elastic coefficients, \( K \) \( (i=S\text{play, Twist, Bend}) \), for uniaxial nematics are proportional to \( S^{-2} \), whereas they involved a third-order contribution proportional to \( S^{-3} \) which removes the degeneracy between \( K_{\text{Splay}} \) and \( K_{\text{Bend}} \) in the Berreman and Meiboom approach[15].

As a future problem it seems to be worthwhile to apply the presently derived TDGL equation in the generalised tensorial form of elastic energy to practical applications of nematodynamics. In addition the flow effect, which was completely ignored at the present stage, is considered to be another challenge to be investigated future.

References