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On the relation between tensor and vector approaches of nematodynamics

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In this paper the relationship between tensorial and vector approaches for elastodynamics is examined in the framework of continuum theory of nematics. It will be elucidated that the Lagrange multipliers are required in the tensorial framework as well as the vector framework to assure equivalence between them. A contraction for the tensorial indices in the time-dependent Ginzburg–Landau equation will be found eventually to result in the vector form concerned with the Ericksen–Leslie equation without flow dynamics.

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1. Introduction

Up to now, 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_i such that $n_i n_i = 1$ and from the Landau–de Gennes phenomenological theory with the tensor order parameter Q_{ij} such that $\mathrm{Tr}\{Q\} = Q_{ii} = 0$ 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]; the latter tensorial approach has been formulated later to involve the hydrodynamics [4, 8]. In spite of the successful applications of these two approaches to a number of practical problems, the theoretical equivalence or relationship between them has not been reported to date even for the simple case without flow effect. 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

$$Q_{ij} = \frac{3}{2} S \left(a_i a_j - \frac{\delta_{ij}}{3} \right) + \frac{B}{2} (b_i b_j - c_i c_j), \qquad (1)$$

where S and B are the microscopic order parameters related to the uniaxial and biaxial orderings of the molecules [9], and the orthonormal triad vector set $\mathbf{a} - \mathbf{b} - \mathbf{c}$ with $\mathbf{a} = \mathbf{n}$, or the director, is assumed hereafter to be the right-handed triad. Recently the present author reported a general expansion approach to derive systematically the elastic free energy expressions of biaxial cholesterics [10] and biaxial smectics [11] in the form of

$$F_e = \frac{1}{2} \sum_{i,j,k,m,n,p} K_{ijkmnp}(\mathbf{a}, \mathbf{b}, \mathbf{c}) Q_{ij,k} Q_{mn,p} + \sum_{i,j,k} D_{ijk}(\mathbf{a}, \mathbf{b}, \mathbf{c}) Q_{ij,k}, \qquad (2)$$

where $K_{ijkmnp}(\mathbf{a}, \mathbf{b}, \mathbf{c})$ and $D_{ijk}(\mathbf{a}, \mathbf{b}, \mathbf{c})$ are the tensorial coefficients, which satisfy symmetry of the system and are to be related to the orthonormal triad basis, or $\mathbf{a} - \mathbf{b} - \mathbf{c}$, and also implicitly involve δ_{ij} and ε_{ijk} [10–13]. The author's expression for the biaxial cholesterics was eventually found to be equivalent to the vector expressions by Brand and Pleiner [14] and also be Govers and Vertogen [15] in the vector formulation. This fact implies that the tensorial expansion according to equation (2) and the vector approach to derive the elastic free energy are substantially equivalent to each other with the relation between the tensor order parameter and the triad as equation (1). In the tensorial approach for uniaxial nematics, a third-order contribution such that $\mathbf{Q}\,\partial\mathbf{Q}\,\partial\mathbf{Q}$ in the tensor order parameter Q_{ij} was given by Berreman and Meiboom [16] to break the degeneracy between the splay and bend elastic constants as seen in the original Landau–de Gennes expansion of the free energy, in which $K_{ijkmnp}(\mathbf{a}, \mathbf{b}, \mathbf{c})$ and $D_{ijk}(\mathbf{a}, \mathbf{b}, \mathbf{c})$ are expanded only in terms of δ_{ij} (Kronecker's δ-function) and ε_{ijk} (Levi–Civita pseudo-tensor).

In a somewhat general approach, the equivalence between the Frank elastic free energy expression and the tensorial form of the uniaxial nematic phase has been first clarified within the second-order expansion of the free energy in terms of the first-order spatial derivative of the tensor order parameter, $Q_{ij,k}$, as well as the

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orthogonal triad, $\mathbf{a}-\mathbf{b}-\mathbf{c}$ [10–13], in order to construct the elastic free energy as an invariant scalar. That is, there exist three independent elastic terms even in the tensorial approach in contrast to the de Gennes pioneering approach [4], in which only two elastic constants in the splay, twist, and bend elastic terms have been found to be independent of each other within the second-order expansion of the elastic free energy in terms of $Q_{ij,k}$. In fact if $K_{ijkmnp}(\mathbf{a},\mathbf{b},\mathbf{c})$ and $D_{ijk}(\mathbf{a},\mathbf{b},\mathbf{c})$ were expanded only in terms of δ_{ij} and ε_{ijk}, one may encounter this degeneracy between the splay and the bend elastic constants.

Assuming a uniaxial cholesteric phase with $B=0$, i.e. the tensor order parameter and its spatial derivatives read

$$Q_{ij}=\frac{3}{2}S\left(a_ia_j-\frac{\delta_{ij}}{3}\right), \tag{3a}$$

and

$$Q_{ij,k}=\frac{3}{2}S(a_ia_j)_{,k}=\frac{3}{2}S(a_{i,k}a_j+a_ia_{j,k}), \tag{3b}$$

respectively, where S is the microscopic order parameter related to the molecular ordering along $\mathbf{n}=\mathbf{a}$ and assumed to be constant in the isothermal equilibrium system under consideration, the explicit form can be given by (see Appendix)

$$\begin{aligned}2F=&L_1\{(b_kQ_{ij,k}a_ib_j)+(c_kQ_{ij,k}a_ic_j)\}^2\\&+L_2\{(b_kQ_{ij,k}a_ic_j)-(c_kQ_{ij,k}a_ib_j)\}^2\\&+L_3\{(a_kQ_{ij,k}a_ib_j)^2+(a_kQ_{ij,k}a_ic_j)^2\}\\&+2L_2q\{(b_kQ_{ij,k}a_ic_j)-(c_kQ_{ij,k}a_ib_j)\}\\=&K_1(n_{i,i})^2+K_2(n_i\varepsilon_{ijk}n_{k,j})^2+K_3n_jn_{i,j}n_kn_{i,k}\\&+2K_2qn_i\varepsilon_{ijk}n_{k,j},\end{aligned} \tag{4}$$

where q is the chiral constant concerned with the natural full pitch P in terms of $q=2\pi/P$, and K_i and L_i are to be related to each other in terms of

$$K_i=\frac{9}{4}S^2L_i \tag{5}$$

($i=1,2,3$ or splay, twist, bend). Here equation (4) is considered to be a general expansion given by equation (2) and may resemble the Berreman and Meiboom approach [16]. In practice, however, since the present expression equation (4) with an orthogonal basis $\mathbf{a}-\mathbf{b}-\mathbf{c}$ in the tensorial coefficients $K_{ijkmnp}(\mathbf{a},\mathbf{b},\mathbf{c})$ and $D_{ijk}(\mathbf{a},\mathbf{b},\mathbf{c})$ is within the second-order in $Q_{ij,k}$, the resultant elastic coefficients, K_i ($i=$ splay, twist, bend), are also quadratic in S as seen in equation (5). In the Berreman and Meiboom approach [16], however, the third-order elastic term in S is involved as a result of the third-order contribution as $\mathbf{Q}\,\partial\mathbf{Q}\,\partial\mathbf{Q}$. From this point, equation (2) or equation (4) may be regarded as a generalized second-order expansion of the elastic free energy in comparison with previous proposals in which $K_{ijkmnp}(\mathbf{a},\mathbf{b},\mathbf{c})$ and $D_{ijk}(\mathbf{a},\mathbf{b},\mathbf{c})$ have been assumed to be expanded only in terms of δ_{ij} and ε_{ijk} instead of the orthogonal basis $\mathbf{a}-\mathbf{b}-\mathbf{c}$ in general. Also equation (4) implies that the tensorial and the vector expressions up to the second-order expansion of $Q_{ij,k}$ have to be equivalent to each other if one starts with the general expansion as equation (2). Even from the viewpoint of the dynamics without any flow effect, the equivalence between the above-mentioned two streams for the continuum theoretical approaches have not yet been clarified.

In this work the mathematical relation between the tensorial and the vector approaches within the framework of the time-dependent Ginzburg–Landau (TDGL) equation is mentioned, with certain restrictions which are accompanied with certain Lagrange multipliers. In §2, the theoretical framework will be mentioned briefly; then §3 and §4 are devoted to some discussion and conclusions, respectively.

2. Theory

In this section let us show the relationship between the tensorial and vector approaches restricting ourselves to the time-dependent Ginzburg–Landau (TDGL) equations.

First of all we have to note the following relation.

$$n_{i,j}=n_k(n_in_k)_{,j}=n_ka_{ik,j}, \tag{6}$$

where the tensor a_{ij} is defined by

$$a_{ij}=n_in_j, \tag{7}$$

or related to Q_{ij} in terms of

$$Q_{ij}=\frac{3}{2}S\left(a_{ij}-\frac{\delta_{ij}}{3}\right), \tag{8}$$

where S is a proportionality constant corresponding to the microscopic molecular ordering. In our consideration, however, S is assumed hereafter to be only a non-vanishing constant.

Noting equation (7), one finds the following identities.

$$\begin{aligned}(n_{i,i})^2=(\delta_{ij}n_{i,j})^2=(\delta_{ij}n_ka_{ik,j})^2=n_kn_ma_{ik,i}a_{jm,j}\\=a_{km}a_{ik,i}a_{jm,j}=a_{kn}a_{mn}a_{ik,i}a_{jm,j},\end{aligned} \tag{9a}$$

$$(\varepsilon_{ijk}n_in_{k,j})^2=(\varepsilon_{ijk}n_in_ma_{mk,j})^2=(\varepsilon_{ijk}a_{im}a_{mk,j})^2, \tag{9b}$$

$$n_jn_{i,j}n_kn_{i,k}=a_{jm}a_{mi,j}a_{kn}a_{ni,k}=a_{jm}a_{kn}a_{mi,j}a_{ni,k}, \tag{9c}$$

where we note the relations

$$a_{ii}=n_in_i=1, \tag{10}$$

$$a_{ij}a_{jk}=a_{ik}. \tag{11}$$

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Then the elastic free energy of uniaxial cholesterics can be derived in terms of $n_{i,j}$ or $a_{ij,k}$

$$\begin{aligned}2F_{\mathrm{e}} &= K_1(n_{i,i})^2 + K_2(n_i\varepsilon_{ijk}n_{k,j})^2 + K_3 n_j n_{i,j} n_k n_{i,k} \\ &\quad + 2K_2 q n_i \varepsilon_{ijk} n_{k,j} \\ &= K_1(a_{kn}a_{mn}a_{ki,i}a_{mj,j}) + K_2(\varepsilon_{ijk}a_{im}a_{mk,j})^2 \\ &\quad + K_3 a_{jm}a_{mi,j}a_{kn}a_{ni,k} + 2K_2 q\varepsilon_{ijk}a_{im}a_{mk,j}. \end{aligned} \tag{12}$$

If we replace $a_{ij,k}$ herein in terms of $Q_{ij,k}$ noting that $S=$ constant, one has an equivalent expression of the same elastic free energy expression as that previously presented by equation (4). Under an electric field E_i, the coupling energy can be simply expressed in terms of

$$F_{\mathrm{E}} = -\frac{1}{2}\varepsilon_a n_i n_j E_i E_j = -\frac{1}{2}\varepsilon_a a_{im}a_{jm}E_iE_j, \tag{13}$$

where we noted equations (7) and (11). Especially, for $K_1=K_2=K_3=K$, equation (12) can be reduced to

$$\begin{aligned}2F_{\mathrm{e}} &= K(n_{i,i})^2 + K(n_{i,j}n_{i,j} - n_{i,j}n_{j,i}) + 2Kqn_i\varepsilon_{ijk}n_{k,j} \\ &= Kn_{i,j}n_{i,j} + 2Kqn_i\varepsilon_{ijk}n_{k,j} + K(n_{j,j}n_i - n_{i,j}n_j)_{,i} \\ &= Kn_{i,j}n_{i,j} + 2Kqn_i\varepsilon_{ijk}n_{k,j} + \text{surface term} \\ &= Ka_{km}a_{ik,j}a_{im,j} + 2Kq\varepsilon_{ijk}a_{im}a_{km,j} + \text{surface term} \\ &= \frac{1}{2}Ka_{ij,k}a_{ij,k} + 2Kq\varepsilon_{ijk}a_{im}a_{km,j} + \text{surface term.} \end{aligned} \tag{14}$$

According to the relations involved to construct the free energy, equations (7), (10), and (11), the constraints for the tensor a_{ij} are given by

$$\mathrm{Tr}(\boldsymbol{a}) = a_{ii} = 1, \tag{15}$$

$$\mathrm{Tr}(\boldsymbol{a}\ \boldsymbol{a}\quad \boldsymbol{a}) = \mathrm{Tr}(\boldsymbol{a}^p) = 1 \qquad (2\leqslant p\leqslant L), \tag{16}$$

$$a_{ij} = a_{ji} \qquad \text{(symmetric)}. \tag{17}$$

Equation (15) stands for a constraint for the conservation of trace of a_{ij} corresponding to equations (7) and (10). Then equation (16) denotes the constraints compatible with $\boldsymbol{a}\ \boldsymbol{a}=\boldsymbol{a}$ or equations (7) and (11), which were involved in the present approach to construct the free energies—equations (12) and (13). Provided that $a_{ij}=n_in_j$ was not included as an *a priori* assumption, then the constraints for each p in equation (16) could be independent of each other. In the present approach, however, the Lagrange multipliers concerned with each $p(2\leqslant p\leqslant L)$ are not independent of each other as will be shown later, since one assumes $a_{ij}=n_in_j$, $a_{ii}=1$, $\boldsymbol{a}\ \boldsymbol{a}=\boldsymbol{a}$, as illustrated in terms of equations (7), (10), and (11).

Now let us define the following functional.

$$\hat{\Pi}_a\{a_{ij}, a_{ij,k}\} = \int_V \mathrm{d}\mathbf{r}\ \Pi_a\{a_{ij}, a_{ij,k}\}, \tag{18}$$

$$\begin{aligned}\Pi_a\{a_{ij}, a_{ij,k}\} &= F - \nu_0 \mathrm{Tr}\{\mathbf{a}\} \\ &\quad - \sum_{p=1}^{L-1}\frac{1}{p+1}\nu_p^*\mathrm{Tr}\{\mathbf{a}^{p+1}\} \\ &\quad - \mu_{ij}(a_{ij}-a_{ji}), \end{aligned} \tag{19}$$

where ν_0, $\nu_p^*(1\leqslant p\leqslant L-1)$, and $\mu_{ij}(1\leqslant i,j\leqslant 3)$ are the Lagrange multipliers related to the previously mentioned constraints on a_{ij} as shown in equations (15) to (17). From the last term in the right-hand side of equation (19), one has to note that μ_{ij} is to be an antisymmetric tensor with three independent components without loss of generality. Therefore the constraints, equations (15) to (17), substantially affect the resultant model to describe the tensor field a_{ij}.

Then the TDGL equation for the tensorial formulation reads

$$\begin{aligned}\gamma_a\frac{\partial a_{ij}}{\partial t} &= -\frac{\delta\hat{\Pi}_a}{\delta a_{ij}} = -\frac{\mathrm{D}\Pi_a}{\mathrm{D}a_{ij}} \\ &= -\frac{\delta\hat{F}}{\delta a_{ij}} + \nu_0\delta_{ij} + \sum_{p=1}^{L-1}\nu_p^*\mathbf{a}_{ij}^p + (\mu_{ij}-\mu_{ji}) \\ &= -\frac{\delta\hat{F}}{\delta a_{ij}} + \nu_0\delta_{ij} + \nu_1 a_{ij} + (\mu_{ij}-\mu_{ji}), \end{aligned} \tag{20}$$

where we noted the relations $a_{ij}=n_in_j$ (see equation (7)) and $\boldsymbol{a}=\boldsymbol{a}\ \boldsymbol{a}$ (see equation (10)), $\delta/\delta a_{ij}$ and $\mathrm{D}/\mathrm{D}a_{ij}$ mean the functional derivative and the Euler differential operation, respectively, γ_a is a viscosity coefficient, and ν_1 is defined by

$$\nu_1 = \sum_{p=1}^{L-1}\nu_p^*, \tag{21}$$

which implies that the constraints expressed by equation (16) for each p are not independent of each other under $a_{ij}=n_in_j$ and $\boldsymbol{a}=\boldsymbol{a}\ \boldsymbol{a}$, but they have to be reduced to the constraint for $p=2$ corresponding to $\mathrm{Tr}\{\boldsymbol{a}^2\}=1$. Therefore the resultant dynamic equation becomes identical to that with $\mathrm{Tr}\{\boldsymbol{a}^2\}=1$ instead of equation (16) in so far as $a_{ij}=n_in_j$ is assumed *a priori*. Hence, since we have five independent constraints corresponding to ν_0, ν_1, μ_{12}, μ_{23}, and μ_{31}, there exist 4 $(=9-5)$ independent components in the tensor field a_{ij}.

Then, in equation (20), $\hat{F}$ is defined as

$$\begin{aligned}\hat{F} &= \int_V \mathrm{d}\mathbf{r}\{F_{\mathrm{e}}(a_{ij}, a_{ij,k}) + F_{\mathrm{E}}(E_i, a_{ij})\} \\ &= \int_V \mathrm{d}\mathbf{r}\{F_{\mathrm{e}}(n_i, n_{i,j}) + F_{\mathrm{E}}(E_i, n_i)\}. \end{aligned} \tag{22}$$

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then the time-dependent Ginzburg–Landau (TDGL) equation (20) leads to

$$\gamma_a \frac{\partial a_{ij}}{\partial t} = h_{ij} + \nu_0 \delta_{ij} + \nu_1 a_{ij} + (\mu_{ij} - \mu_{ji}) \qquad (1 \leqslant i, j \leqslant 3), \tag{23}$$

where the tensorial molecular field, h_{ij}, is defined by

$$h_{ij} = -\frac{\partial F}{\partial a_{ij}} + \left(\frac{\partial F}{\partial a_{ij,k}} \right)_{,k}. \tag{24}$$

Hence we have five unknowns, ν_0, ν_1, μ_{12}, μ_{23}, and μ_{31} corresponding to the constraints, or equations (15) to (17), in the tensor a_{ij} with nine components in general. Therefore only four ($=2\times 2$) components in a_{ij} are independent of each other which is found to be consistent with such a constraint as $a_{ij} = n_i n_j$, or $\boldsymbol{a} = \boldsymbol{n} \otimes \boldsymbol{n}$ (the direct product of $\boldsymbol{n}$), in which each $\boldsymbol{n}$ has two independent components because of $\boldsymbol{n}\ \boldsymbol{n} = 1$. From equation (23), noting that $a_{ij} = a_{ji}$, one may readily find

$$\gamma_a \frac{\partial a_{ij}}{\partial t} = h_{(ij)} + \nu_0 \delta_{ij} + \nu_1 a_{ij}, \tag{25a}$$

$$0 = h_{[ij]} + (\mu_{ij} - \mu_{ji}) = h_{[ij]} + 2\mu_{[ij]} = h_{[ij]} + 2\mu_{ij}, \tag{25b}$$

where the effective symmetric $h_{(ij)}$ and skew symmetric molecular field components $h_{[ij]}$ are defined by

$$h_{(ij)} = \frac{1}{2}(h_{ij} + h_{ji}), \tag{26a}$$

and

$$h_{[ij]} = \frac{1}{2}(h_{ij} - h_{ji}), \tag{26b}$$

respectively. Equation (25a), which involves two unknown Lagrange multipliers, i.e. ν_0 and ν_1, consists of four ($=6-2$) independent equations. On the other hand, equation (25b) results in the relation to determine three unknowns, i.e. μ_{12}, μ_{23}, and μ_{31}. In practice, from equation (25b), the unknown antisymmetric tensor components μ_{ij} are given by

$$\mu_{ij} = -\frac{1}{2} h_{[ij]} = -\frac{1}{4}(h_{ij} - h_{ji}). \tag{27}$$

It has to be noted here that the tensor a_{ij} remains symmetric as far as a_{ij} is assumed to be symmetric as an initial condition and μ_{ij} is given by equation (27). In practice if one substitutes equation (27) into equation (23) and notes equation (26a), then equation (25a) can be easily obtained.

Now if one takes account of the following identity,

$$\delta_{ij} = a_i a_j + b_i b_j + c_i c_j = a_{ij} + b_i b_j + c_i c_j, \tag{28}$$

equation (25a) can be rewritten as

$$\gamma_a \frac{\partial a_{ij}}{\partial t} = h_{(ij)} + \nu a_{ij} + \lambda_{ij}, \tag{29}$$

where

$$\nu = \nu_0 + \nu_1, \tag{30a}$$

and

$$\lambda_{ij} = \nu_0 (b_i b_j + c_i c_j) = \lambda_{ji}. \tag{30b}$$

It should be noted here that νa_{ij} and λ_{ij} may be regarded as tensor components parallel to a_{ij} and orthogonal to it, respectively. From the definition of equation (30b), λ_{ij} may be regarded as a uniaxially symmetric tensor about n_i as a principal axis.

Now let us determine the unknowns, ν_0 and ν_1, which may be certain functions of time, t as well as space, $\mathbf{r}$. In practice, noting that $a_{ij} = a_{ji}$, one may readily derive

$$3\nu_0 + \nu_1 = -h_{(ii)} = -h_{ii}, \tag{31a}$$

$$\nu_0 + \nu_1 = -a_{ij} h_{(ij)} = -a_{ij} h_{ij}, \tag{31b}$$

or

$$\nu_0 = \frac{1}{2}(a_{ij} - \delta_{ij}) h_{ij}, \tag{32a}$$

$$\nu_1 = \frac{1}{2}(\delta_{ij} - 3a_{ij}) h_{ij}. \tag{32b}$$

Thus substituting equation (32a) into equations (30a) and (30b), one finds

$$\nu = \nu_0 + \nu_1 = -a_{ij} h_{ij}, \tag{33a}$$

$$\lambda_{ij} = \frac{1}{2}(a_{mn} - \delta_{mn}) h_{mn} (\delta_{ij} - a_{ij}). \tag{33b}$$

Now we are at the position to derive the vector expression of the TDGL equation from the tensor expression, equation (25a). Multiplying n_j in both sides of equation (25a), one has straightforwardly

$$\gamma_a \frac{\partial n_i}{\partial t} = n_j h_{(ij)} + \nu n_i. \tag{34}$$

Then the unknown ν can be determined in terms of

$$\nu = -n_i n_j h_{(ij)} = -a_{ij} h_{(ij)} = -a_{ij} h_{ij} = a_{ij} \frac{\delta F}{\delta a_{ij}}, \tag{35}$$

which is found to coincide with equation (31b). From

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equations (12) and (13), equation (24) reads

$$h_{ij} = \left\{ -\frac{\partial F}{\partial a_{ij}} + \left(\frac{\partial F}{\partial a_{ij,k}} \right)_k \right\}$$
$$= K \left\{ -q\varepsilon_{ikm} a_{mj,k} + \frac{1}{2} a_{ij,kk} + q\varepsilon_{mki} a_{mj,k} \right\} + \frac{1}{2}\varepsilon_a E_i E_j$$
$$= K \left\{ \frac{1}{2} a_{ij,kk} - 2q\varepsilon_{ikm} a_{mj,k} \right\} + \frac{1}{2}\varepsilon_a E_i E_j. \quad (36)$$

On the other hand, if one makes use of the vector expression for the elastic free energy equations (12) and (13), within the constraint on the director n_i instead of equations (15) to (17),

$$n_i n_i = 1. \quad (37)$$

Then the functional $\Pi_n\{n_i, n_{ij}\}$ may be introduced in the same manner as equaton (19), i.e.

$$\Pi_n\{n_i, n_{i,j}\} = F\{n_i, n_{i,j}\} - \frac{1}{2}\eta n_i n_i, \quad (38)$$

$$\hat{\Pi}_n\{n_i, n_{i,j}\} = \int_V \mathrm{d}\mathbf{r}\, \Pi_n\{n_i, n_{i,j}\}, \quad (39)$$

where η is the Lagrange multiplier corresponding to equation (37) [17].

Hence one has the following TDGL equation.

$$\gamma \frac{\partial n_i}{\partial t} = -\frac{\delta \hat{\Pi}_n}{\delta n_i} = h_i + \eta n_i, \quad (40)$$

where γ is the Leslie viscosity coefficient [7], and the molecular field h_i is defined by

$$h_i = -\frac{\delta \hat{F}}{\delta n_i} = -\frac{\partial F}{\partial n_i} + \left(\frac{\partial F}{\partial n_{i,j}} \right)_j. \quad (41)$$

For one constant approximation concerned with the elastic constants, one has the following molecular field.

$$h_i = Kn_{i,kk} + 2Kq\varepsilon_{ijk} n_{k,j} + \varepsilon_a E_i E_j n_j$$
$$= K(n_m a_{im,k})_{,k} + 2Kq\varepsilon_{ijk} n_m a_{km,j} + \varepsilon_a E_i E_j n_j$$
$$= K(n_p a_{mp,k} a_{im,k} + n_m a_{im,kk})$$
$$+ 2Kq\varepsilon_{ijk} n_m a_{km,j} + \varepsilon_a E_i E_j n_j. \quad (42)$$

From equation (40), the unknown η has to be determined by

$$\eta = -n_i h_i. \quad (43)$$

From comparison between equations (34) and (40), one finds the following relations on the viscosity coefficients and the Lagrange multipliers.

$$\gamma = 2\gamma_a, \quad (44)$$

$$h_i + \eta n_i = 2(n_j h_{(ij)} + \nu n_i). \quad (45)$$

The above relations imply that both h_i and h_{ij} may be accompanied with some uncertainties corresponding to the above-mentioned constraints upon them.

Let us derive the tensorial expression from the vector expression, or equation (40) below. First of all, to obtain a tensorial expression, multiplying by n_j on both sides of equation (40), one has

$$\gamma n_j \frac{\partial n_i}{\partial t} = h_i n_j + \eta n_i n_j. \quad (46a)$$

Exchanging a couple of indices, i and j, in the above expression, one readily obtains

$$\gamma n_i \frac{\partial n_j}{\partial t} = h_j n_i + \eta n_i n_j. \quad (46b)$$

From equations (46 a) and (46 b), one readily finds

$$\gamma_a \frac{\partial a_{ij}}{\partial t} = \frac{1}{2}(h_i n_j + h_j n_i) + \eta a_{ij}. \quad (47)$$

Thus one finds

$$\gamma_a \frac{\partial a_{ij}}{\partial t} = h_{(ij)} + \nu a_{ij} + \lambda_{ij}$$
$$= \frac{1}{2}(n_i h_j + n_j h_i) + \eta a_{ij}. \quad (48)$$

Hence we have the following relation between h_i and h_{ij},

$$\frac{1}{2}(h_i n_j + h_j n_i) = h_{(ij)} + \lambda_{ij} + (\nu - \eta) a_{ij}$$
$$= h_{(ij)} + \nu_0(\delta_{ij} - a_{ij}) + (\nu_0 + \nu_1 - \eta) a_{ij}$$
$$= h_{(ij)} + \nu_0 \delta_{ij} + (\nu_1 - \eta) a_{ij}. \quad (49a)$$

The above identity implies that there exist uncertainties both parallel to a_{ij} ($(\nu - \eta)a_{ij}$ term in equation (49 a)) and perpendicular to it (λ_{ij} term in equation (49 a)) concerning the relation between the tensorial molecular field, $h_{(ij)}$, and the vector field, h_i, through n_i. Now multiplying by n_j on both sides of equation (49 a) and noting that $\lambda_{ij} n_j = 0$, one readily derives

$$h_i = 2n_j h_{(ij)} + 2(\nu - \eta) n_i - n_j h_j n_i$$
$$= 2n_j h_{(ij)} + 2(\nu - \eta) n_i + \eta n_i$$
$$= 2n_j h_{(ij)} + (2\nu - \eta) n_i, \quad (49b)$$

which coincides with equation (45) previously derived.

To end this section, it seems instructive to note that one may derive the tensor expression for dynamics from the vector expression and *vice versa*, taking account of

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appropriate Lagrange multipliers concerned with the constraints on the field.

3. Discussion

In this work, we have examined the relation between the director and the tensor expressions for nematodynamics. A similar argument had been reported by Kilian and Hess [18] and recently by Sonnet *et al.* [19]. Ignoring the previously noted constraints for the tensor order parameter

$$Q_{ij}\left[=\frac{3}{2}S\left(a_{ij}-\frac{\delta_{ij}}{3}\right)\right]$$

or a_{ij}, they had proposed the following tensorial expression instead of equation (23) [18],

$$\gamma_a\frac{\partial a_{ij}}{\partial t}=h_{ij}+\Phi_{ij}, \tag{50}$$

where Φ_{ij}, is defined by [16]

$$\Phi_{ij}=-\frac{\delta F_0}{\delta a_{ij}}; \tag{51}$$

here F_0 is the isotropic part of the free energy expanded phenomenologically up to the fourth-order in a_{ij} as [4]

$$\begin{aligned}F_0&=\frac{A(T)}{2}S^2\mathrm{Tr}\{a^2\}+\frac{B}{3}S^3\mathrm{Tr}\{a^3\}+\frac{C}{4}S^4\mathrm{Tr}\{a^4\}\\&=\frac{A(T)}{2}S^2+\frac{B}{3}S^3+\frac{C}{4}S^4,\end{aligned} \tag{52}$$

with

$$A(T)=A_0(T-T_c)\qquad(A_0>0), \tag{53}$$

$$B<0, \tag{54}$$

$$C>0, \tag{55}$$

where T_c is a critical temperature related to the nematic–isotropic phase transition [4, 5]. Hence we have the following relation

$$\begin{aligned}\Phi_{ij}&=-\frac{\delta F_0}{\delta a_{ij}}\\&=-\{A(T)Sa_{ij}+BS^2(a^2)_{ij}+CS^3(a^3)_{ij}\}\\&=-\{A(T)S+BS^2+CS^3\}a_{ij}\\&=-A^\dagger(T)a_{ij},\end{aligned} \tag{56}$$

where we defined $A^\dagger(T)$ as follows:

$$A^\dagger(T)=A(T)S+BS^2+CS^3. \tag{57}$$

From the above relation, the temperature dependence of the microscopic order parameter S can be determined by the minimized free energy which corresponds to a certain global minimum of F_0 at a given T. Then one may readily derive,

$$\gamma_a\frac{\partial a_{ij}}{\partial t}=h_{ij}-A^\dagger a_{ij}. \tag{58}$$

Then, making use of the constraint on a_{ij} expressed by

$$\mathrm{Tr}\{\mathbf{a}^2\}=1, \tag{59}$$

we have the following relation from equation (50),

$$A^\dagger=a_{ij}h_{ij}. \tag{60}$$

At first sight, one may see that this relation may resemble equation (35) for the Lagrange multiplier ν. However it has to be borne in mind that the left-hand side of equation (60) is to be determined by the invariant scalars, which are independent of the elastic deformations involved in equation (56), whereas the right-hand side comes from the elastic property of nematics and the coupling energy with the external fields (see equations (12) and (13)). Therefore equation (60) can no longer be satisfied in general if one does not take account of the Lagrange multipliers introduced in the present approach, i.e. ν_0 and ν_1 in equation (25*a*). They also claimed that since $A^\dagger(T)=0$ around an equilibrium point, one may ignore Φ_{ij} in the dynamic equation (50) [18]. In practice they introduced the following simplified form as the basic dynamic equation instead of equation (50) [19].

$$\gamma_a\frac{\partial a_{ij}}{\partial t}=h_{ij}. \tag{61}$$

From this one has the following constraint for a_{ij} and h_{ij} to satisfy equation (61),

$$a_{ij}h_{ij}=0, \tag{62}$$

which implies orthogonality between a_{ij} and h_{ij}. In general, however, this relation cannot be the case for a general expression of the molecular field defined by equation (24).

In conclusion we have to note that the Lagrange multipliers must be involved as in equation (23) so as to investigate the dynamics in the tensorial form. Especially, without $\nu=\nu_0+\nu_1$ related to η in equation (45), we can no longer derive the vector form from the tensorial one with some reduction of the tensors, since η has somehow to be related to ν as given in equation (49*a*).

4. Conclusions

In this paper we have proposed a TDGL equation of nematodynamics in a tensorial form, which is consistent with the constraints for the tensor a_{ij} as given in equations (15) to (17), taking certain Lagrange multipliers into account. It has been found that the Lagrange multipliers are required to support the relation between the tensorial and vector approaches. In addition we have presented an explicit tensorial expression for the Frank

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elastic free energy with three independent elastic constants on the basis of an extended second-order expansion in terms of $Q_{ij,k}$ as defined by equation (2). Therein it should be noted that such degeneracy between the splay and the bend elastic constants as presented in previous works [4, 5] can be removed within the second-order expansion of $a_{ij,k}$ or $Q_{ij,k}$ by including the orthogonal basis $\mathbf{a}-\mathbf{b}-\mathbf{c}$ into the tensorial expansion coefficients $K_{ijkmnp}(\mathbf{a},\mathbf{b},\mathbf{c})$ and $D_{ijk}(\mathbf{a},\mathbf{b},\mathbf{c})$ in equation (1) in a similar manner to that in previous work related to biaxial cholesterics and smectics [10–13]. In such an extended approach, all elastic coefficients, K_i (i = splay, 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_{Splay} and K_{Bend} in the Berreman and Meiboom approach [16].

As a future problem it seems to be worthwhile to apply the presently derived TDGL equation in the generalized tensorial form 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 in the future.

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Appendix

First, we have to note the following relations:

$$b_k Q_{ij,k} a_i b_j = \frac{3}{2} S b_k (a_i a_{j,k} + a_{i,k} a_j) a_i b_j = \frac{3}{2} S b_k a_{j,k} b_j, \tag{A1}$$

$$c_k Q_{ij,k} a_i c_j = \frac{3}{2} S c_k (a_i a_{j,k} + a_{i,k} a_j) a_i c_j = \frac{3}{2} S c_k a_{j,k} c_j, \tag{A2}$$

$$b_k Q_{ij,k} a_i c_j = \frac{3}{2} S b_k (a_i a_{j,k} + a_{i,k} a_j) a_i c_j = \frac{3}{2} S b_k a_{j,k} c_j, \tag{A3}$$

$$c_k Q_{ij,k} a_i b_j = \frac{3}{2} S c_k (a_i a_{j,k} + a_{i,k} a_j) a_i c_j = \frac{3}{2} S c_k a_{j,k} b_j, \tag{A4}$$

$$a_k Q_{ij,k} a_i b_j = \frac{3}{2} S a_k (a_i a_{j,k} + a_{i,k} a_j) a_i b_j = \frac{3}{2} S a_k a_{j,k} b_j, \tag{A5}$$

$$a_k Q_{ij,k} a_i c_j = \frac{3}{2} S a_k (a_i a_{j,k} + a_{i,k} a_j) a_i c_j = \frac{3}{2} S a_k a_{j,k} c_j. \tag{A6}$$

Also the following vector formulae are available:

$$\begin{aligned} a_{i,i} &= a_{i,j}\delta_{i,j} \\ &= a_{i,j}(a_i a_j + b_i b_j + c_i c_j) \\ &= a_{i,j}(b_i b_j + c_i c_j) \\ &= b_j a_{i,j} b_i + c_j a_{i,j} c_j, \end{aligned} \tag{A7}$$

$$\begin{aligned} a_i \varepsilon_{ijk} a_{k,j} &= (b_j c_k - c_j b_k) a_{k,j} \\ &= b_j a_{k,j} c_k - c_j a_{k,j} b_k, \end{aligned} \tag{A8}$$

$$\begin{aligned} a_j a_{i,j} a_k a_{i,k} &= a_j a_{i,j} a_k a_{m,k} \delta_{im} \\ &= a_j a_{i,j} a_k a_{m,k} (a_i a_m + b_i b_m + c_i c_m) \\ &= a_j a_{i,j} a_k a_{m,k} (b_i b_m + c_i c_m) \\ &= a_j a_{i,j} b_i a_k a_{m,k} b_m + a_j a_{i,j} c_i a_k a_{m,k} c_m \\ &= (a_j a_{i,j} b_i)^2 + (a_j a_{i,j} c_i)^2. \end{aligned} \tag{A9}$$

From equations (A2) to (A9) one readily finds equations (4) and (5).

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