Journal of Applied Mechanics and Technical Physics, Vol. 48, No. 2, pp. 229–240, 2007

ORIENTATION MECHANICS OF LIQUID CRYSTALS. TRANSITION TO A LOCAL COORDINATE SYSTEM

S. I. Trashkeev

UDC 532.783

Equations of orientation mechanics of liquid crystals, written in a local rotational coordinate system related to the director orientation, are considered. A condition is obtained, which ensures qualitative similarity between solutions predicted by an approximate (single-constant) model and solutions obtained with the original formulation of the problem. Equations that provide a more exact approximation to the general model are proposed. The use of matrices in recording of energy relations allows a fairly easy transition to other coordinate systems and studying more sophisticated models for the description of the orientation state of liquid crystals. A transition to a local coordinate system makes it possible to compute three-dimensional liquid-crystal structures on moderate-performance personal computers.

Key words: *liquid crystal, mechanics of continuous media, rotation groups.*

Introduction. Equations that describe the state of liquid crystals (LC) follow from the continuum theory of mechanics of anisotropic liquids. The Ericksen–Leslie approach has been most comprehensively developed and is widely used in studying the liquid-crystal state [1, 2]. Previously, many phenomena that occur in liquid crystals could be considered with the use of a one- or two-dimensional (normally, in the linear approximation) model with deformation of LC orientation in one plane. Currently, this is insufficient. The need in considering more complicated models is primarily determined by the development of nanotechnologies [3] based on studying polymer and liquid-crystal composites [4, 5]. When new properties of such composites are described, a three-dimensional problem is often posed, which have to be solved to determine the orientation state of a liquid crystal containing small-scale or point defects.

Though the Ericksen–Leslie theory has been finalized, derivation of the full system of equilibrium equations for the LC director is rather cumbersome. Such a procedure (e.g., with the use of the MAPLE symbolic language, otherwise errors are possible) for a three-dimensional nematic liquid crystal (NLC) without allowance for hydrodynamics yields a system of equations that will take several pages to be recorded. In this case, even a preliminary analysis does not seem possible. A matrix formalism whose basic mathematical postulates are borrowed from mechanics of continuous media [6, 7] is proposed in the present paper. In a theoretical study, this approach allows one to use many postulates of the algebra of rotation groups SU(2), SO(3) [8] and to write the final equations in a rather compact form, substantially facilitating both the preliminary analysis and the transition to other coordinate systems. A model that describes orientation interactions in the liquid crystal (without allowance for liquid motion) is considered.

Continuum Equations. For an incompressible isothermal anisotropic liquid, the basic unknowns are the velocity field $\boldsymbol{v} = \boldsymbol{v}(t, \boldsymbol{r})$, the director $\boldsymbol{n} = \boldsymbol{n}(t, \boldsymbol{r})$ (for a uniaxial medium), and the pressure $p(t, \boldsymbol{r})$ [t is the time and $\boldsymbol{r} = (x, y, z) \equiv (x_1, x_2, x_3)$ is the radius vector in the Cartesian coordinate system]. The system of equations for finding $\boldsymbol{n}$, $\boldsymbol{v}$, and p can be written in the form [2]

Institute of Laser Physics, Siberian Division, Russian Academy of Sciences, Novosibirsk 630090; sitrskv@mail.ru. Translated from Prikladnaya Mekhanika i Tekhnicheskaya Fizika, Vol. 48, No. 2, pp. 98–111, March–April, 2007. Original article submitted May 3, 2006.

$$\frac{\partial}{\partial x_j}\,\frac{\partial F}{\partial\,(\partial n_i/\partial x_j)}-\frac{\partial F}{\partial n_i}-\lambda n_i=I\,\frac{\partial^2 n_i}{\partial t^2}+\gamma_1\Big(\frac{\partial n_i}{\partial t}-V_{ij}n_j\Big)+\gamma_2 n_j\Omega_{ji},$$

$$\operatorname{div}\boldsymbol{v}=\frac{\partial v_j}{\partial x_j}=0, \tag{1}$$

$$\rho\Big(\frac{\partial v_i}{\partial t}+v_j\,\frac{\partial v_i}{\partial x_j}\Big)=f_i+\frac{\partial\Sigma_{ji}}{\partial x_j},$$

where $\lambda=\lambda(t,\boldsymbol{r})$ is the Lagrangian factor, which provides the fulfillment of the normalization condition $\boldsymbol{n}^2=1$; F, I, and ρ are the density of free energy, density of the moment of inertia, and mass density of the NLC, respectively, f_i are the components of the bulk force density vector, Σ_{ji} is the stress tensor. Summation is performed over repeated indices if not indicated otherwise. In the variants of LC interaction with external fields under consideration, we may neglect the contribution of ponderomotive or strictional forces to f_j [2] and assume that

$$f_j=-\frac{\partial p}{\partial x_j}\qquad(\boldsymbol{f}=-\nabla p),$$

where p is the ambient pressure. The stress tensor is the sum of the elastic (terms depending on F) and viscous parts:

$$\Sigma_{ij}=-\frac{\partial F}{\partial\,(n_k/\partial x_i)}\,\frac{\partial n_k}{\partial x_j}+\mu_1 n_i n_j\Omega_{km}n_k n_m+\mu_2 n_i\Big(\frac{\partial n_j}{\partial t}-V_{jk}n_k\Big)$$

$$+\mu_3 n_j\Big(\frac{\partial n_i}{\partial t}-V_{ik}n_k\Big)+\mu_4\Omega_{ij}+\mu_5 n_i n_k\Omega_{kj}+\mu_6\Omega_{ik}n_k n_j$$

($\mu_1,\ldots,\mu_6$ are the viscous Leslie coefficients and $\gamma_1=\mu_3-\mu_2$ and $\gamma_2=\mu_6-\mu_5$). The components of the velocity-gradient tensor are written as

$$\Omega_{ij}=\frac{1}{2}\Big(\frac{\partial v_i}{\partial x_j}-\frac{\partial v_j}{\partial x_i}\Big),\qquad V_{ij}=\frac{1}{2}\Big(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i}\Big).$$

The density of free energy F is determined by internal elastic forces depending on n_i, on the gradients $\partial n_i/\partial x_j$, and on the parameters of external forcing. If F is considered as a functional, the left side of the first equation of system (1) is the Lagrangian variation in terms of the variables n_i and $\partial n_i/\partial x_j$ [1, 2].

If we introduce the quantity $\bar F$ as

$$\bar F=F-I\Big(\frac{\partial\boldsymbol{n}}{\partial t}\Big)^2, \tag{2}$$

where $I(\partial\boldsymbol{n}/\partial t)^2$ is the rotational kinetic energy, and vary $\bar F$ with respect to an additional variable $\partial n_i/\partial t$, the overall variation takes the form

$$\frac{\delta\bar F}{\delta n_i}=\frac{\partial}{\partial t}\,\frac{\partial\bar F}{\partial\,(\partial n_i/\partial t)}+\frac{\partial}{\partial x_j}\,\frac{\partial\bar F}{\partial\,(\partial n_i/\partial x_j)}-\frac{\partial\bar F}{\partial n_i}-\lambda n_i=0, \tag{3}$$

where

$$\frac{\partial}{\partial t}\,\frac{\partial\bar F}{\partial\,(\partial n_i/\partial t)}=-I\,\frac{\partial^2 n_i}{\partial t^2}.$$

The remaining equations of system (1) are written in the previous form with the substitution $F\to\bar F$. In the general form, the functional $\bar F$ with the opposite sign is an analog of the Lagrangian for rotational motion of a solid in analytical mechanics.

Matrix Form of the Expression for Free Energy. To derive the equations, we choose the Cartesian coordinate system and use the following notation: $\theta=\theta(t,\boldsymbol{r})$ and $\varphi=\varphi(t,\boldsymbol{r})$ are the polar and azimuthal angles, respectively, which are related to $\boldsymbol{n}$ by

$$\boldsymbol{n}=(n_x,n_y,n_z)=(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta). \tag{4}$$

To simplify the computations, the following notation is reasonable:

$$S_\theta=\sin\theta,\qquad C_\theta=\cos\theta,\qquad S_\varphi=\sin\varphi,\qquad C_\varphi=\cos\varphi,$$

$$\boldsymbol{m} = (m_x, m_y, m_z) = \frac{\partial \boldsymbol{n}}{\partial \theta} = (C_\theta C_\varphi, C_\theta S_\varphi, -S_\theta),$$
$$\boldsymbol{p} = (p_x, p_y, p_z) = \frac{1}{S_\theta}\frac{\partial \boldsymbol{n}}{\partial \varphi} = (-S_\varphi, C_\varphi, 0), \tag{5}$$
$$(\boldsymbol{nm}) = 0, \qquad (\boldsymbol{np}) = 0, \qquad (\boldsymbol{mp}) = 0$$

($\boldsymbol{m}$ and $\boldsymbol{p}$ are additional unit vectors orthogonal to $\boldsymbol{n}$). The directions $\boldsymbol{n}$, $\boldsymbol{m}$, and $\boldsymbol{p}$ form the right triplet of vectors and satisfy the following relations:

$$[\boldsymbol{mp}] = \boldsymbol{n}, \qquad [\boldsymbol{pn}] = \boldsymbol{m}, \qquad [\boldsymbol{nm}] = \boldsymbol{p}. \tag{6}$$

In the case of a strained state of the NLC or a cholesteric liquid crystal (CLC) with the absence of polarity (equivalence of the directions $\boldsymbol{n}$ and $-\boldsymbol{n}$), the expression for the density of free energy F is written as the sum of several terms that take into account different types of interaction in the medium [1]. Taking into account Eq. (2) and omitting the bar over F, we write the relation

$$F = -F_k + F_{\rm el} + F_E + F_d + F_{sf}, \tag{7}$$

where

$$F_{\rm el} = (1/2)\{K_1(\operatorname{div}\boldsymbol{n})^2 + K_2(\boldsymbol{n}\operatorname{rot}\boldsymbol{n} + q_0)^2 + K_3[\boldsymbol{n}\operatorname{rot}\boldsymbol{n}]^2\},$$
$$F_k = I\Big(\frac{\partial \boldsymbol{n}}{\partial t}\Big)^2, \qquad F_E = -\frac{\varepsilon_a}{8\pi}(\boldsymbol{nE})^2, \qquad F_d = -(\boldsymbol{PE}). \tag{8}$$

We introduce the notation for potential energy: $F_p = F_{\rm el} + F_E + F_d$. Here F_k and $F_{\rm el}$ are the rotational kinetic and elastic energies, F_E and F_d are the anisotropic (electrostatic) and flexoelectric (dipole) contributions to the energy of LC interaction with the electric field $\boldsymbol{E} = \boldsymbol{E}(t, \boldsymbol{r})$, K_1, K_2, and K_3 are the Frank constants, $q_0 = 2\pi/h_0$ is the wavenumber of an undisturbed CLC ($q_0 = 0$ refers to the nematic state), h_0 is the pitch, $\varepsilon_a = \varepsilon_{||} - \varepsilon_\perp$, where $\varepsilon_{||}$ and $\varepsilon_\perp$ are the parameters of the dielectric permeability tensor, which is expressed via the Cartesian components of the director n_i in the form

$$\varepsilon_{ij} = \varepsilon_\perp \delta_{ij} + \varepsilon_a n_i n_j, \qquad i, j = \{x, y, z\}$$

(δ_{ij} is the Kronecker delta). The vector $\boldsymbol{P}$ (density of the dipole moment) has the form [2]

$$\boldsymbol{P} = e_1 \boldsymbol{n} \operatorname{div}\boldsymbol{n} - e_3[\boldsymbol{n}\operatorname{rot}\boldsymbol{n}],$$

where e_1 and e_3 are the flexoelectric coefficients. The contribution of the surface part of the energy F_{sf} in the final equations is taken into account by the boundary conditions for the director $\boldsymbol{n}$; therefore, F_{sf} need not be defined explicitly in the present work. The total free energy is determined by the volume and surface integrals

$$F_{\rm tot} = \int\limits_V F\, dv + \int\limits_S F_{sf}\, ds \tag{9}$$

(V is the LC volume and S is the area bounding the volume).

The equations of orientation motion determining the dependence $\boldsymbol{n} = \boldsymbol{n}(t, \boldsymbol{r})$ are derived from system (1) with $\boldsymbol{v} \equiv 0$ or by minimization of the total free energy (9) with respect to all variations of the director $\boldsymbol{n}$ (3) and phenomenological allowance for the relaxation term with the first derivative with respect to time. As a result, we obtain a relation of the form [2]

$$I\frac{\partial^2 n_j}{\partial t^2} + \gamma_1 \frac{\partial n_j}{\partial t} = \frac{\partial}{\partial x_i}\frac{\partial F}{\partial(\partial n_j/\partial x_i)} - \frac{\partial F}{\partial n_j} - \lambda n_j,$$
$$\lambda(t, \boldsymbol{r}) = -I\frac{\partial n_j}{\partial t}\frac{\partial n_j}{\partial t} + \Big(n_j \frac{\partial}{\partial x_i}\frac{\partial F}{\partial(\partial n_j/\partial x_i)} - n_j\frac{\partial F}{\partial n_j}\Big). \tag{10}$$

In using the variational approach for obtaining dissipative equations of motion in the absence of hydrodynamic flows, one can use a more rigorous (than phenomenological) approach based on introducing a relaxation potential [9]. In the steady-state case, where the unknowns are independent of time, Eq. (10) acquires the form

$$0 = \frac{\partial}{\partial x_i}\,\frac{\partial F}{\partial\,(\partial n_j/\partial x_i)} - \frac{\partial F}{\partial n_j} - \lambda n_j, \tag{11}$$

whereby

$$\lambda(t,\boldsymbol{r}) = n_j\Big(\frac{\partial}{\partial x_i}\,\frac{\partial F}{\partial\,(\partial n_j/\partial x_i)} - \frac{\partial F}{\partial n_j}\Big).$$

Within the framework of the trigonometric presentation of the director $\boldsymbol{n}$ (2), it is not necessary to introduce the Lagrangian factor, because the normalization conditions are satisfied automatically. Then the variational relation (10) transforms to a system of equations for the angles θ and φ:

$$\begin{aligned}
\frac{\delta F}{\delta\theta} &= \frac{\partial}{\partial t}\,\frac{\partial F}{\partial\,(\partial\theta/\partial t)} + \gamma_1\,\frac{\partial\theta}{\partial t} - \frac{\partial}{\partial x_i}\,\frac{\partial F}{\partial\,(\partial\theta/\partial x_i)} + \frac{\partial F}{\partial\theta} = 0,\\
\frac{\delta F}{\delta\varphi} &= \frac{\partial}{\partial t}\,\frac{\partial F}{\partial\,(\partial\varphi/\partial t)} + \gamma_1 S_\theta^2\,\frac{\partial\varphi}{\partial t} - \frac{\partial}{\partial x_i}\,\frac{\partial F}{\partial\,(\partial\varphi/\partial x_i)} + \frac{\partial F}{\partial\varphi} = 0.
\end{aligned} \tag{12}$$

Equations (10)–(12) have to be supplemented by the boundary conditions for $\boldsymbol{n}$ or θ and φ at points on S. Substituting Eqs. (4), (5) into the expression for the elastic part of the density of free energy $F_{\rm el}$, we obtain the following relation from Eq. (8):

$$F_{\rm el} = \frac{K_1}{2}\,[(\boldsymbol{m}\nabla\theta) + S_\theta(\boldsymbol{p}\nabla\varphi)]^2 + \frac{K_2}{2}\,[-(\boldsymbol{p}\nabla\theta) + S_\theta(\boldsymbol{m}\nabla\varphi) + q_0]^2 + \frac{K_3}{2}\,[\boldsymbol{m}(\boldsymbol{n}\nabla\theta) + S_\theta\boldsymbol{p}(\boldsymbol{n}\nabla\varphi)]^2.$$

The expression for $F_{\rm el}$ can be reasonably written as the sum of the nematic part ($q_0 = 0$) and an additive determining the cholesteric order ($q_0 \neq 0$):

$$F_{\rm el} = F_{\rm el}^0 + F_{\rm el}^h.$$

Here

$$F_{\rm el}^0 = \frac{K_1}{2}\,[(\boldsymbol{m}\nabla\theta) + S_\theta(\boldsymbol{p}\nabla\varphi)]^2 + \frac{K_2}{2}\,[-(\boldsymbol{p}\nabla\theta) + S_\theta(\boldsymbol{m}\nabla\varphi)]^2 + \frac{K_3}{2}\,[\boldsymbol{m}(\boldsymbol{n}\nabla\theta) + S_\theta\boldsymbol{p}(\boldsymbol{n}\nabla\varphi)]^2, \tag{13}$$

$$F_{\rm el}^h = K_2 q_0(\boldsymbol{n}\,\mathrm{rot}\,\boldsymbol{n}) = K_2 q_0[-(\boldsymbol{p}\nabla\theta) + S_\theta(\boldsymbol{m}\nabla\varphi)].$$

Similar trigonometric substitutions for $\boldsymbol{P}$ and F_d yield the relations

$$\boldsymbol{P} = e_1\boldsymbol{n}[(\boldsymbol{m}\nabla\theta) + S_\theta(\boldsymbol{p}\nabla\varphi)] + e_3[\boldsymbol{m}(\boldsymbol{n}\nabla\theta) + S_\theta\boldsymbol{p}(\boldsymbol{n}\nabla\varphi)].$$

Then, we obtain

$$F_d = -e_1(\boldsymbol{n}\boldsymbol{E})[(\boldsymbol{m}\nabla\theta) + S_\theta(\boldsymbol{p}\nabla\varphi)] - e_3[(\boldsymbol{m}\boldsymbol{E})(\boldsymbol{n}\nabla\theta) + S_\theta(\boldsymbol{p}\boldsymbol{E})(\boldsymbol{n}\nabla\varphi)].$$

The electric part of free energy remains unchanged, and the kinetic term F_k transforms to

$$F_k = \frac{I}{2}\Big[\Big(\frac{\partial\theta}{\partial t}\Big)^2 + S_\theta^2\Big(\frac{\partial\varphi}{\partial t}\Big)^2\Big] = \frac{I}{2}\left(\dot\theta^2 + S_\theta^2\dot\varphi^2\right). \tag{14}$$

Let us consider the expression for the elastic part of free energy of the nematic ($q_0 = 0$) $F_{\rm el}^0$. Developing the quadratures, we obtain

$$\begin{aligned}
F_{\rm el}^0 &= \frac{K_1}{2}\,[(\boldsymbol{m}\nabla\theta)^2 + S_\theta^2(\boldsymbol{p}\nabla\varphi)^2] + \frac{K_2}{2}\,[(\boldsymbol{p}\nabla\theta)^2 + S_\theta^2(\boldsymbol{m}\nabla\varphi)^2]\\
&+ \frac{K_3}{2}\,[(\boldsymbol{n}\nabla\theta)^2 + S_\theta^2(\boldsymbol{n}\nabla\varphi)^2] + S_\theta[K_1(\boldsymbol{m}\nabla\theta)(\boldsymbol{p}\nabla\varphi) - K_2(\boldsymbol{p}\nabla\theta)(\boldsymbol{m}\nabla\varphi)].
\end{aligned} \tag{15}$$

We can write the cross term in Eq. (15) in a symmetric form if we use the vector identity

$$S_\theta[(\boldsymbol{m}\nabla\theta)(\boldsymbol{p}\nabla\varphi) - (\boldsymbol{m}\nabla\varphi)(\boldsymbol{p}\nabla\theta)] = S_\theta(\boldsymbol{n}[\nabla\theta\nabla\varphi]) \tag{16}$$

and take into account that the complex in the right side of Eq. (16) does not contribute to variation (12):

$$\frac{\delta}{\delta\theta}\,S_\theta(\boldsymbol{n}[\nabla\theta\nabla\varphi]) = \frac{\delta}{\delta\varphi}\,S_\theta(\boldsymbol{n}[\nabla\theta\nabla\varphi]) = \frac{\delta}{\delta\theta}\,(\boldsymbol{n}[\nabla\theta\nabla\varphi]) = \frac{\delta}{\delta\varphi}\,(\boldsymbol{n}[\nabla\theta\nabla\varphi]) = 0. \tag{17}$$

The resultant expression for $F_{\rm el}^0$ takes the form

$$F_{\rm el}^0 = \frac{K_1}{2}\,[(\boldsymbol{m}\nabla\theta)^2 + S_\theta^2(\boldsymbol{p}\nabla\varphi)^2] + \frac{K_2}{2}\,[(\boldsymbol{p}\nabla\theta)^2 + S_\theta^2(\boldsymbol{m}\nabla\varphi)^2]$$

$$+\,\frac{K_3}{2}\,[(\boldsymbol{n}\nabla\theta)^2 + S_\theta^2(\boldsymbol{n}\nabla\varphi)^2] + \frac{K_1-K_2}{2}\,S_\theta[(\boldsymbol{m}\nabla\theta)(\boldsymbol{p}\nabla\varphi) + (\boldsymbol{p}\nabla\theta)(\boldsymbol{m}\nabla\varphi)]. \tag{18}$$

For the single-constant case, where $K_1 = K_2 = K_3 = K$, Eq. (13) for $F_{\rm el} = F_{\rm el}^0 + F_{\rm el}^h$ transforms to the expression

$$F_{\rm el} = (K/2)[(\nabla\theta)^2 + S_\theta^2(\nabla\varphi)^2] + Kq_0[-(\boldsymbol{p}\nabla\theta) + S_\theta(\boldsymbol{m}\nabla\varphi)],$$

whose variation is written as

$$\frac{\delta F_{\rm el}}{\delta\theta} = K[\Delta\theta - S_\theta C_\theta(\nabla\varphi)^2 + 2q_0 S_\theta(\boldsymbol{n}\nabla\varphi)],$$

$$\frac{\delta F_{\rm el}}{\delta\varphi} = K[\mathrm{div}\,(S_\theta^2\nabla\varphi) - 2q_0 S_\theta(\boldsymbol{n}\nabla\theta)]. \tag{19}$$

The variation of the kinetic energy is found in a similar manner:

$$\frac{\delta F_k}{\delta\theta} = \frac{\partial}{\partial t}\,\frac{\partial F_k}{\partial\,(\partial\theta/\partial t)} - \frac{\partial F_k}{\partial\theta} = I\Big[\frac{\partial^2\theta}{\partial t^2} - S_\theta C_\theta\Big(\frac{\partial\varphi}{\partial t}\Big)^2\Big],$$

$$\frac{\delta F_k}{\delta\varphi} = \frac{\partial}{\partial t}\,\frac{\partial F_k}{\partial\,(\partial\varphi/\partial t)} - \frac{\partial F_k}{\partial\varphi} = I\,\frac{\partial}{\partial t}\Big(S_\theta^2\,\frac{\partial\varphi}{\partial t}\Big). \tag{20}$$

According to Eqs. (19) and (20), the equations of orientation motion of the director with allowance for the relaxation term in the absence of external forcing acquire the form of nonlinear hyperbolic equations for decaying waves [7]:

$$I(\ddot\theta - S_\theta C_\theta\dot\varphi^2) + \gamma_1\dot\theta = K[\Delta\theta - S_\theta C_\theta(\nabla\varphi)^2 + 2q_0 S_\theta(\boldsymbol{n}\nabla\varphi)],$$

$$I\,\frac{\partial}{\partial t}\,(S_\theta^2\dot\varphi) + \gamma_1 S_\theta^2\dot\varphi = K\,\mathrm{div}\,[S_\theta^2\nabla\varphi - 2q_0 S_\theta(\boldsymbol{n}\nabla\theta)] \tag{21}$$

(the dot indicates the derivative with respect to time).

The equations of motion in a trigonometric form (21) for negligibly low inertia are given in [10]. For $I \approx 0$, Eqs. (21) transform to a system of nonlinear parabolic equations of the type of heat-conduction or diffusion equations [7]. In the above-mentioned papers and in [11–13], interaction of bounded light beams with nematic liquid crystals ($q_0 = 0$) was considered by means of numerical computations. Zharkova and Trashkeev [14] considered a particular case of steady-state equations (21) for computing the orientation structure of a cholesteric liquid crystal ($q_0 \neq 0$) in a spherical capsule. Equations in the form (21) are fairly simple, and their solutions in most cases do not differ from the exact description of the orientation structures of liquid crystals. Such a statement is normally given without proof [1]. An analysis of this situation requires a detailed consideration of both approaches.

We write Eq. (18) in the matrix form

$$F_{\rm el}^0 = \frac{1}{2}\Big(\frac{\partial\theta}{\partial x_i}\,T_{ij}\,\frac{\partial\theta}{\partial x_j} + S_\theta^2\,\frac{\partial\varphi}{\partial x_i}\,\Phi_{ij}\,\frac{\partial\varphi}{\partial x_j} + (K_1 - K_2)\,S_\theta\frac{\partial\theta}{\partial x_i}\,\Lambda_{ij}\,\frac{\partial\varphi}{\partial x_j}\Big), \tag{22}$$

where

$$[T_{ij}] = \begin{pmatrix} (K_1C_\theta^2 + K_3S_\theta^2)C_\varphi^2 + K_2S_\varphi^2 & (K_1C_\theta^2 + K_3S_\theta^2 - K_2)S_\varphi C_\varphi & (K_3 - K_1)S_\theta C_\theta C_\varphi \\ (K_1C_\theta^2 + K_3S_\theta^2 - K_2)S_\varphi C_\varphi & (K_1C_\theta^2 + K_3S_\theta^2)S_\varphi^2 + K_2C_\varphi^2 & (K_3 - K_1)S_\theta C_\theta S_\varphi \\ (K_3 - K_1)S_\theta C_\theta C_\varphi & (K_3 - K_1)S_\theta C_\theta S_\varphi & K_1S_\theta^2 + K_3C_\theta^2 \end{pmatrix}; \tag{23}$$

$$[\Phi_{ij}] = \begin{pmatrix} (K_2C_\theta^2 + K_3S_\theta^2)C_\varphi^2 + K_1S_\varphi^2 & (K_2C_\theta^2 + K_3S_\theta^2 - K_1)S_\varphi C_\varphi & (K_3 - K_2)S_\theta C_\theta C_\varphi \\ (K_2C_\theta^2 + K_3S_\theta^2 - K_1)S_\varphi C_\varphi & (K_2C_\theta^2 + K_3S_\theta^2)S_\varphi^2 + K_1C_\varphi^2 & (K_3 - K_2)S_\theta C_\theta S_\varphi \\ (K_3 - K_2)S_\theta C_\theta C_\varphi & (K_3 - K_2)S_\theta C_\theta S_\varphi & K_2S_\theta^2 + K_3C_\theta^2 \end{pmatrix}; \tag{24}$$

$$[\Lambda_{ij}] = \begin{pmatrix} -2C_\theta C_\varphi S_\varphi & C_\theta(C_\varphi^2 - S_\varphi^2) & S_\theta S_\varphi \\ C_\theta(C_\varphi^2 - S_\varphi^2) & 2C_\theta C_\varphi S_\varphi & -S_\theta C_\varphi \\ S_\theta S_\varphi & -S_\theta C_\varphi & 0 \end{pmatrix}. \tag{25}$$

The matrices $T = [T_{ij}]$, $\Phi = [\Phi_{ij}]$, and $\Lambda = [\Lambda_{ij}]$ are symmetric. The elastic free energy is presented as the sum of two quadratic forms of the gradients $\partial\theta/\partial x_i$ and $\partial\varphi/\partial x_i$ and the biquadratic form of the same gradients. The quantities T, Φ, and Λ can be presented via orthogonal matrices [6] as

$$T = Q^{\mathrm{t}}\tilde{T}Q, \qquad \Phi = Q^{\mathrm{t}}\tilde{\Phi}Q, \qquad \Lambda = Q^{\mathrm{t}}\tilde{\Lambda}Q, \qquad \det Q = 1,$$

where the superscript "t" means transposition,

$$Q = [Q_{ij}] = \begin{pmatrix} m_x & m_y & m_z \\ p_x & p_y & p_z \\ n_x & n_y & n_z \end{pmatrix} = \begin{pmatrix} C_\theta C_\varphi & C_\theta S_\varphi & -S_\theta \\ -S_\varphi & C_\varphi & 0 \\ S_\theta C_\varphi & S_\theta S_\varphi & C_\theta \end{pmatrix}. \tag{26}$$

This matrix obeys the orthogonality expression $Q^{-1} = Q^{\mathrm{t}}$. Thereby, the matrices $\tilde{T}$, $\tilde{\Phi}$, and $\tilde{\Lambda}$ take the form

$$\tilde{T} = \begin{pmatrix} K_1 & 0 & 0 \\ 0 & K_2 & 0 \\ 0 & 0 & K_3 \end{pmatrix}, \qquad \tilde{\Phi} = \begin{pmatrix} K_2 & 0 & 0 \\ 0 & K_1 & 0 \\ 0 & 0 & K_3 \end{pmatrix}, \qquad \tilde{\Lambda} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

If we write the biquadratic term in the expression for elastic free energy without symmetrization with the use of Eq. (16), we obtain another expression equivalent for the variation

$$F^0_{\mathrm{el}} = \frac{1}{2}\Big(\frac{\partial\theta}{\partial x_i}\,T_{ij}\,\frac{\partial\theta}{\partial x_j} + S^2_\theta\,\frac{\partial\varphi}{\partial x_i}\,\Phi_{ij}\,\frac{\partial\varphi}{\partial x_j} + 2S_\theta\,\frac{\partial\theta}{\partial x_i}\,\Pi_{ij}\,\frac{\partial\varphi}{\partial x_j}\Big),$$

where the matrix Π can be presented in the form

$$\Pi = Q^{\mathrm{t}}\tilde{\Pi}Q = Q^{\mathrm{t}}\begin{pmatrix} 0 & K_1 & 0 \\ -K_2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}Q.$$

According to [6], the matrices $\tilde{T}$, $\tilde{\Phi}$, and $(K_1 - K_2)\tilde{\Lambda}$ are strain tensors; the matrix Q is responsible for rotation in a three-dimensional Euclidean space, because $\det Q = 1$, and can be presented as the product of two orthogonal matrices

$$Q = NM, \qquad N = \begin{pmatrix} C_\theta & 0 & -S_\theta \\ 0 & 1 & 0 \\ S_\theta & 0 & C_\theta \end{pmatrix}, \qquad M = \begin{pmatrix} C_\varphi & S_\varphi & 0 \\ -S_\varphi & C_\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Here $N = N(\theta)$, $M = M(\varphi)$, and $Q = Q(\theta, \varphi)$ are the elements of the rotation group SO(3) [8] by the angles θ and φ.

A similar presentation is written for the remaining terms of the potential part in the expression for free energy (7), (8):

$$F_E = -\frac{\varepsilon_a}{8\pi}\,(\boldsymbol{nE})^2 = -\frac{\varepsilon_a}{8\pi}\,E_i L_{ij} E_j, \qquad L = Q^{\mathrm{t}}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}Q; \tag{27}$$

$$F_d = -(\boldsymbol{PE}) = -E_i A_{ij}\,\frac{\partial\theta}{\partial x_j} - S_\theta E_i B_{ij}\,\frac{\partial\varphi}{\partial x_j}. \tag{28}$$

Here

$$A = [A_{ij}] = \begin{pmatrix} (e_1+e_3)S_\theta C_\theta C^2_\varphi & (e_1+e_3)S_\theta C_\theta S_\varphi C_\varphi & C_\varphi(e_3C^2_\theta - e_1S^2_\theta) \\ (e_1+e_3)S_\theta C_\theta S_\varphi C_\varphi & (e_1+e_3)S_\theta C_\theta S^2_\varphi & S_\varphi(e_3C^2_\theta - e_1S^2_\theta) \\ C_\varphi(e_1C^2_\theta - e_3S^2_\theta) & S_\varphi(e_1C^2_\theta - e_3S^2_\theta) & -(e_1+e_3)S_\theta C_\theta \end{pmatrix}; \tag{29}$$

$$B = [B_{ij}] = \begin{pmatrix} -(e_1+e_3)S_\theta S_\varphi C_\varphi & S_\theta(e_1C^2_\varphi - e_3S^2_\varphi) & -e_3C_\theta S_\varphi \\ S_\theta(e_3C^2_\varphi - e_1S^2_\varphi) & (e_1+e_3)S_\theta S_\varphi C_\varphi & e_3C_\theta C_\varphi \\ -e_1C_\theta S_\varphi & e_1C_\theta C_\varphi & 0 \end{pmatrix}. \tag{30}$$

After orthogonal expansion, the matrices A and B become

$$A = Q^{\mathrm{t}}\tilde{A}Q, \quad \tilde{A} = \begin{pmatrix} 0 & 0 & e_3 \\ 0 & 0 & 0 \\ e_1 & 0 & 0 \end{pmatrix}, \qquad B = Q^{\mathrm{t}}\tilde{B}Q, \quad \tilde{B} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & e_3 \\ 0 & e_1 & 0 \end{pmatrix}.$$

The additive to the density of free energy F^h_{el} due to allowance for the cholesteric order is written as the sum

$$F^h_{\mathrm{el}} = K_2 q_0 \Big(- p_i \frac{\partial \theta}{\partial x_i} + S_\theta m_i \frac{\partial \varphi}{\partial x_i} \Big). \tag{31}$$

Thus, the original expression for the density of free energy (7), (8) is presented as linear, quadratic, and biquadratic forms in a factorized form with respect to the variational variables θ, φ, $\dot{\theta}$, $\dot{\varphi}$, $\partial\theta/\partial x_i$, and $\partial\varphi/\partial x_i$.

Apart from Eq. (17), other commutation relations are also valid, which satisfy the zero variation and are obtained by cyclic permutation of unit vectors. In addition to Eq. (16), we can write the expressions

$$\begin{gathered} g_1 \equiv (\boldsymbol{p}\nabla\theta)(\boldsymbol{n}\nabla\varphi) - (\boldsymbol{p}\nabla\varphi)(\boldsymbol{n}\nabla\theta) = (\boldsymbol{m}[\nabla\theta\nabla\varphi]), \\ g_2 \equiv (\boldsymbol{n}\nabla\theta)(\boldsymbol{m}\nabla\varphi) - (\boldsymbol{n}\nabla\varphi)(\boldsymbol{m}\nabla\theta) = (\boldsymbol{p}[\nabla\theta\nabla\varphi]), \\ g_3 \equiv (\boldsymbol{m}\nabla\theta)(\boldsymbol{p}\nabla\varphi) - (\boldsymbol{m}\nabla\varphi)(\boldsymbol{p}\nabla\theta) = (\boldsymbol{n}[\nabla\theta\nabla\varphi]), \\ \boldsymbol{G} \equiv [\nabla\theta\nabla\varphi] \end{gathered} \tag{32}$$

for which the following conditions are satisfied:

$$\frac{\delta g_1}{\delta\theta} = \frac{\delta g_1}{\delta\varphi} = 0, \qquad \frac{\delta g_2}{\delta\theta} = \frac{\delta g_2}{\delta\varphi} = 0, \qquad \frac{\delta g_3}{\delta\theta} = \frac{\delta g_3}{\delta\varphi} = 0,$$

$$\frac{\delta\,(\boldsymbol{GG})}{\delta\theta} = \frac{\delta\,(\boldsymbol{GG})}{\delta\varphi} = 0, \qquad \frac{\delta G_i}{\delta\theta} = \frac{\delta G_i}{\delta\varphi} = 0, \qquad i = \{x, y, z\}.$$

Variation (12) of all terms F (7) in the matrix form can now be performed; the result will be presented in a comparatively compact form, because all variables are separated, and differentiation is trivial. The derivatives of the introduced matrices are calculated as follows:

$$\frac{\partial T}{\partial\theta} = 2M^{\mathrm{t}}N^{\mathrm{t}}\tilde{T}\,\frac{\partial N}{\partial\theta}\,M = 2M^{\mathrm{t}}\,\frac{\partial N^{\mathrm{t}}}{\partial\theta}\,\tilde{T}NM, \qquad \frac{\partial T}{\partial\varphi} = 2M^{\mathrm{t}}N^{\mathrm{t}}\tilde{T}N\,\frac{\partial M}{\partial\varphi} = 2\,\frac{\partial M^{\mathrm{t}}}{\partial\varphi}\,N^{\mathrm{t}}\tilde{T}NM. \tag{33}$$

Here

$$\frac{\partial N}{\partial\theta} = \begin{pmatrix} -S_\theta & 0 & -C_\theta \\ 0 & 0 & 0 \\ C_\theta & 0 & -S_\theta \end{pmatrix}, \qquad \frac{\partial M}{\partial\varphi} = \begin{pmatrix} -S_\varphi & C_\varphi & 0 \\ -C_\varphi & -S_\varphi & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

The calculations for the remaining matrices Φ, L, A, and B are performed in a similar manner by substituting them instead of T into Eq. (33). Nevertheless, the computational procedure and the final form of the equations remain rather cumbersome. For a more compact form, we propose replacement of variables, similar to that used in mechanics of continuous media in the transition from the Eulerian to the Lagrangian coordinates [6]. The possibility of using such a transition to curvilinear coordinates was indicated long ago by Ericksen [2], but no detailed analysis with indication of a particular form of the conversion has not been performed until now.

Transition to a Local Coordinate System. The quadratic form of recording the expression for free energy with the use of matrices allows us to pass to a curvilinear local coordinate system

$$(x, y, z) \equiv (x_1, x_2, x_3) \to (\xi_1, \xi_2, \xi_3) \equiv (\xi, \eta, \zeta) \tag{34}$$

by means of the transformation

$$\frac{\partial \xi_i}{\partial x_j} = Q_{ij}, \qquad \xi_i = \int Q_{ij}\,dx_j + C_i,$$

where, according to the rules of the vector analysis, $\boldsymbol{C} = (C_1, C_2, C_3)$ is a vector function equal to the rotors of another arbitrary vector function [7, 9] determined in each particular case and depending on the form of the

boundary conditions. For Eq. (34) to exist, the Jacobian of transformation has to be other than zero. Taking into account the definition of Q as a rotation matrix (26), we obtain

$$\frac{\partial\,(\xi_1,\xi_2,\xi_3)}{\partial\,(x_1,x_2,x_3)} = \det\left[\frac{\partial\xi_i}{\partial x_j}\right] = \det Q = 1.$$

In the new variables $(\xi_1,\xi_2,\xi_3) \equiv (\xi,\eta,\zeta)$, the components of free energy are written as

$$F_{\rm el}^0 = (1/2)[K_1\theta_\xi^2 + K_2\theta_\eta^2 + K_3\theta_\zeta^2 + S_\theta^2(K_2\varphi_\xi^2 + K_1\varphi_\eta^2 + K_3\varphi_\zeta^2)] + (K_1 - K_2)S_\theta(\theta_\xi\varphi_\eta + \theta_\eta\varphi_\xi).$$

Here the Greek subscripts at θ and φ indicate differentiation with respect to the corresponding coordinates. The kinetic term F_k remains unchanged (14). The cholesteric, dielectric, and flexoelectric additives acquire the form

$$F_{\rm el}^h = K_2 q_0(-\theta_\eta + S_\theta\varphi_\xi),$$

$$F_E = -\varepsilon_a E_\zeta^2/(8\pi), \qquad F_d = -e_1E_\zeta(\theta_\xi + S_\theta\varphi_\eta) - e_3(E_\xi\theta_\zeta + S_\theta E_\eta\varphi_\zeta),$$

where

$$\begin{pmatrix} E_\xi \\ E_\eta \\ E_\zeta \end{pmatrix} = Q\begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix} = \begin{pmatrix} C_\theta C_\varphi & C_\theta S_\varphi & -S_\theta \\ -S_\varphi & C_\varphi & 0 \\ S_\theta C_\varphi & S_\theta S_\varphi & C_\theta \end{pmatrix}\begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}. \tag{35}$$

In the case of variation of free energy written in the original coordinate system, the electric field vector $\boldsymbol{E}$ is assumed to be independent of the variational variables [15]. In the case of the transition to local coordinates, according to Eq. (35), we have to take into account the conditions and properties following from the definition of the unit vectors (4)–(6), namely,

$$\frac{\partial\,(\boldsymbol{mE})}{\partial\theta} = -(\boldsymbol{nE}), \qquad \frac{\partial\,(\boldsymbol{mE})}{\partial\varphi} = C_\theta(\boldsymbol{pE}), \qquad \frac{\partial\,(\boldsymbol{pE})}{\partial\theta} = 0, \qquad \frac{\partial\,(\boldsymbol{pE})}{\partial\varphi} = (\boldsymbol{lE}),$$

$$\frac{\partial\,(\boldsymbol{nE})}{\partial\theta} = (\boldsymbol{mE}), \qquad \frac{\partial\,(\boldsymbol{nE})}{\partial\varphi} = S_\theta(\boldsymbol{pE})$$

or

$$\frac{\partial E_\xi}{\partial\theta} = -E_\zeta, \qquad \frac{\partial E_\xi}{\partial\varphi} = C_\theta E_\eta, \qquad \frac{\partial E_\eta}{\partial\theta} = 0, \qquad \frac{\partial E_\eta}{\partial\varphi} = -S_\theta E_\xi - C_\theta E_\zeta,$$

$$\frac{\partial E_\zeta}{\partial\theta} = E_\xi, \qquad \frac{\partial E_\zeta}{\partial\varphi} = S_\theta E_\eta.$$

The operation of divergence, which is necessary to compute the variational relations, acquires the following form in the local coordinate system:

$$\operatorname{div}\boldsymbol{Z} \to \widetilde{\operatorname{div}}\tilde{\boldsymbol{Z}} + Z_\xi(-\theta_\zeta + C_\theta\varphi_\eta) - Z_\eta(C_\theta\varphi_\xi + S_\theta\varphi_\zeta) + Z_\zeta(\theta_\xi + S_\theta\varphi_\eta)$$

[$\boldsymbol{Z}$ and $\tilde{\boldsymbol{Z}} = (Z_\xi, Z_\eta, Z_\zeta)$ are arbitrary differentiable vectors in the original and local coordinate systems, respectively]. To simplify the relations, it is reasonable to introduce the vector $\boldsymbol{\chi} = \boldsymbol{\chi}(x,y,z) \to \tilde{\boldsymbol{\chi}} = \tilde{\boldsymbol{\chi}}(\xi,\eta,\zeta)$. Then, the expressions for potential energy variation in the local coordinate system become

$$\frac{\delta F_p}{\delta\theta} = \frac{\partial}{\partial x_i}\frac{\partial F_p}{\partial\,(\partial\theta/\partial x_i)} - \frac{\partial F_p}{\partial\theta} \to \frac{\partial}{\partial\xi_i}\frac{\partial F_p}{\partial\,(\partial\theta/\partial\xi_i)} + \tilde{\chi}_i\frac{\partial F_p}{\partial\,(\partial\theta/\partial\xi_i)} - \frac{\partial F_p}{\partial\theta},$$

$$\frac{\delta F_p}{\delta\varphi} = \frac{\partial}{\partial x_i}\frac{\partial F_p}{\partial\,(\partial\varphi/\partial x_i)} - \frac{\partial F_p}{\partial\varphi} \to \frac{\partial}{\partial\xi_i}\frac{\partial F_p}{\partial\,(\partial\varphi/\partial\xi_i)} + \tilde{\chi}_i\frac{\partial F_p}{\partial\,(\partial\varphi/\partial\xi_i)} - \frac{\partial F_p}{\partial\varphi}.$$

Here

$$\tilde{\boldsymbol{\chi}} \to Q\boldsymbol{\chi},$$

$$\boldsymbol{\chi} \equiv (\chi_x,\chi_y,\chi_z) = \boldsymbol{m}\operatorname{div}\boldsymbol{m} + \boldsymbol{p}\operatorname{div}\boldsymbol{p} + \boldsymbol{n}\operatorname{div}\boldsymbol{n}$$

$$= \boldsymbol{m}[-(\boldsymbol{n}\nabla\theta) + C_\theta(\boldsymbol{p}\nabla\varphi)] - \boldsymbol{p}[C_\theta(\boldsymbol{m}\nabla\varphi) + S_\theta(\boldsymbol{n}\nabla\varphi)] + \boldsymbol{n}[(\boldsymbol{m}\nabla\theta) + S_\theta(\boldsymbol{p}\nabla\varphi)],$$

$$\tilde{\boldsymbol{\chi}} \equiv (\chi_\xi,\chi_\eta,\chi_\zeta) \equiv (-\theta_\zeta + C_\theta\varphi_\eta, -C_\theta\varphi_\xi - S_\theta\varphi_\zeta, \theta_\xi + S_\theta\varphi_\eta);$$

the tilde means that the corresponding operation is performed in the local coordinate system, and the vectors in performing the transformation have to be written in the form of columns.

The resultant relations allow us to perform variation and to find expressions for orientation motion of the director. Thus, the contribution of the elastic part of free energy is written as

$$\frac{\delta F^0_{\rm el}}{\delta\theta} = K_1[\theta_{\xi\xi} + C_\theta\varphi_\eta(\theta_\xi - S_\theta\varphi_\eta)] + K_2[\theta_{\eta\eta} - \theta_\eta(C_\theta\varphi_\xi + S_\theta\varphi_\zeta) + S_\theta\varphi_\xi(S_\theta\varphi_\zeta - C_\theta\varphi_\xi)]$$

$$+ K_3[\theta_{\zeta\zeta} + S_\theta\theta_\zeta\varphi_\eta - S_\theta\varphi_\zeta(S_\theta\varphi_\xi + C_\theta\varphi_\zeta)] + (K_1 - K_2)S_\theta(\varphi_{\xi\eta} + C_\theta\varphi^2_\eta),$$

$$\frac{\delta F^0_{\rm el}}{\delta\varphi} = K_1\Big[\frac{\partial}{\partial\eta}\,(S^2_\theta\varphi_\eta) - C_\theta\theta_\eta\theta_\xi\Big] + K_2\Big[\frac{\partial}{\partial\xi}\,(S^2_\theta\varphi_\xi) + (C_\theta\theta_\xi + S_\theta\theta_\zeta)\theta_\eta - S^2_\theta\varphi_\xi\theta_\zeta\Big] \tag{36}$$

$$+ K_3\Big[\frac{\partial}{\partial\zeta}\,(S^2_\theta\varphi_\zeta) - S_\theta\theta_\eta\theta_\zeta + S^2_\theta\varphi_\zeta\theta_\xi\Big] + (K_1 - K_2)\Big[\frac{\partial}{\partial\eta}\,(S_\theta\theta_\xi) - S_\theta C_\theta\theta_\eta\varphi_\eta\Big].$$

The additive due to the cholesteric order becomes

$$\frac{\delta F^h_{\rm el}}{\delta\theta} = 2K_2q_0S_\theta\varphi_\zeta, \qquad \frac{\delta F^h_{\rm el}}{\delta\varphi} = -2K_2q_0S_\theta\theta_\zeta. \tag{37}$$

The variations of the dielectric (F_E) and flexoelectric (F_d) terms are written as

$$\frac{\delta F_E}{\delta\theta} = \frac{\varepsilon_a}{4\pi}\,E_\xi E_\zeta, \qquad \frac{\delta F_E}{\delta\varphi} = \frac{\varepsilon_a}{4\pi}\,S_\theta E_\eta E_\zeta; \tag{38}$$

$$\frac{\delta F_d}{\delta\theta} = e_1\Big(E_\xi(\theta_\xi + S_\theta\varphi_\eta) - \frac{\partial E_\zeta}{\partial\xi}\Big) + e_3\Big(E_\eta(C_\theta\varphi_\zeta + S_\theta\varphi_\xi) - E_\zeta\theta_\zeta - S_\theta E_\xi\varphi_\eta - \frac{\partial E_\xi}{\partial\zeta}\Big),$$

$$\frac{\delta F_d}{\delta\varphi} = e_1S_\theta\Big(E_\eta(\theta_\xi + S_\theta\varphi_\eta) - \frac{\partial E_\zeta}{\partial\eta}\Big) + e_3S_\theta\Big(E_\xi\theta_\eta - E_\eta\theta_\xi - (C_\theta E_\xi + S_\theta E_\zeta)\varphi_\zeta - \frac{\partial E_\eta}{\partial\zeta}\Big). \tag{39}$$

Thus, a system of equations for orientation motion of the NLC and CLC director in a local coordinate system is obtained. In considering the corresponding interaction, we have to sum up the variational relations (20), (36)–(39), which allow us to take into account the influence of external geometric and internal configurational conditions, as well as electric fields, in a fairly general statement. Using a similar approach, we can consider more complicated models of the functional of free energy (7), (8), which take into account higher (than quadratic) terms of expansion, for example, the elastic Nehring–Saupe model [16] or a model including quadrupole interaction with electric fields [17].

Single-Constant Approximation. Let us determine to which extent the description of the orientation structure on the basis of the single-constant approximation agrees with the model that takes into account the difference in all elastic coefficients under strain. The following comment should be preliminary made. If differentiation is considered as an action of certain operators, we can formally write

$$\begin{pmatrix} \partial/\partial\xi \\ \partial/\partial\eta \\ \partial/\partial\zeta \end{pmatrix} \leftrightarrow Q \begin{pmatrix} \partial/\partial x \\ \partial/\partial y \\ \partial/\partial z \end{pmatrix} \leftrightarrow \begin{pmatrix} (\boldsymbol{m}\nabla) \\ (\boldsymbol{p}\nabla) \\ (\boldsymbol{n}\nabla) \end{pmatrix}; \tag{40}$$

in this case, the procedure of the transition from one coordinate system to another is reduced to simple replacement of the corresponding operators in accordance with Eq. (40). The resultant variational relations transform to similar relations written in the original coordinate system.

To analyze the single-constant case, we write the elastic part of variation of free energy (36) under the condition $K_1 = K_2 = K_3 = K$. We obtain

$$\frac{\delta F^0_{\rm el}}{\delta\theta} = K\Big[\tilde\Delta\theta - S_\theta C_\theta(\tilde\nabla\varphi)^2 + C_\theta\tilde g_3 - S_\theta\tilde g_1\Big], \qquad \frac{\delta F^0_{\rm el}}{\delta\varphi} = K\Big[\widetilde{\rm div}\,(S^2_\theta\tilde\nabla\varphi) - S^2_\theta\tilde g_2\Big]. \tag{41}$$

Here the tilde means that the corresponding operation is performed in the local coordinate system. The vector $\tilde{\boldsymbol{g}} = (\tilde g_1, \tilde g_2, \tilde g_3) = (g_\xi, g_\eta, g_\zeta)$ is the vector product in the local coordinate system

$$\tilde{\boldsymbol{g}} = [\tilde\nabla\theta\tilde\nabla\varphi] = (\theta_\eta\varphi_\zeta - \theta_\zeta\varphi_\eta, -\theta_\xi\varphi_\zeta + \theta_\zeta\varphi_\xi, \theta_\xi\varphi_\eta - \theta_\eta\varphi_\xi)$$

and is related to the above-introduced vectors $\boldsymbol{g}$ and $\boldsymbol{G}$ (32) by the transformation relation

$$\tilde{\boldsymbol{g}} \to \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix} = Q[\nabla\theta\nabla\varphi] = Q\boldsymbol{G} = \begin{pmatrix} (\boldsymbol{m}\boldsymbol{G}) \\ (\boldsymbol{p}\boldsymbol{G}) \\ (\boldsymbol{n}\boldsymbol{G}) \end{pmatrix}.$$

Equalities (41) written in the original coordinate system transform to Eq. (19) at $q_0 = 0$. Thereby, we have to take into account the vector identities, which follow from the definition of the unit vectors (4) and (5),

$$\tilde{\Delta}\theta \to (\boldsymbol{m}\nabla(\boldsymbol{m}\nabla\theta)) + (\boldsymbol{p}\nabla(\boldsymbol{p}\nabla\theta)) + (\boldsymbol{n}\nabla(\boldsymbol{n}\nabla\theta)) = \Delta\theta - \theta_x\varphi_y + \theta_y\varphi_x = \Delta\theta - G_z,$$

$$\tilde{\Delta}\varphi \to (\boldsymbol{m}\nabla(\boldsymbol{m}\nabla\varphi)) + (\boldsymbol{p}\nabla(\boldsymbol{p}\nabla\varphi)) + (\boldsymbol{n}\nabla(\boldsymbol{n}\nabla\varphi))$$

$$= \Delta\varphi + S_\varphi(\theta_y\varphi_z - \theta_z\varphi_y) + C_\varphi(\theta_z\varphi_x - \theta_x\varphi_z) = \Delta\varphi + S_\theta G_x + C_\theta G_y,$$

$$(\tilde{\nabla}\theta)^2 \to (\boldsymbol{m}\nabla\theta)^2 + (\boldsymbol{p}\nabla\theta)^2 + (\boldsymbol{n}\nabla\theta)^2 = (\nabla\theta)^2,$$

$$(\tilde{\nabla}\varphi)^2 \to (\boldsymbol{m}\nabla\varphi)^2 + (\boldsymbol{p}\nabla\varphi)^2 + (\boldsymbol{n}\nabla\varphi)^2 = (\nabla\varphi)^2,$$

and the definition of the components of the vector product $\boldsymbol{G} = [\nabla\theta\nabla\varphi]$. According to Eq. (32), we can write

$$\boldsymbol{G} = \boldsymbol{m}(\boldsymbol{m}\boldsymbol{G}) + \boldsymbol{p}(\boldsymbol{p}\boldsymbol{G}) + \boldsymbol{n}(\boldsymbol{n}\boldsymbol{G}) = g_1\boldsymbol{m} + g_2\boldsymbol{p} + g_3\boldsymbol{n},$$

$$C_\theta g_3 - S_\theta g_2 = G_z, \qquad C_\varphi G_y - S_\varphi G_x = g_2,$$

$$\boldsymbol{G} \equiv [\nabla\theta\nabla\varphi] = (\theta_y\varphi_z - \theta_z\varphi_y, -\theta_x\varphi_z + \theta_z\varphi_x, \theta_x\varphi_y - \theta_y\varphi_x).$$

Note that the quantities g_1, g_2, and g_3 and the components of the vector $\boldsymbol{G}$ under variation make a zero contribution to the equations of motion. In other words, they are functions of coordinates only and do not explicitly depend on time. By analogy with the definitions of analytical mechanics, they may be called integrals of motion, whose values are determined by correlated initial and boundary conditions. This fact is important in integrating the equations of motion and particularly important in the numerical implementation. The use of the above-derived integrals of motion yields a severalfold reduction of the computational time and computer memory.

In addition to the quantities g_i and G_i, we can indicate several more integrals of motion, including an external action, which are based on considering the free energy functional as a certain generalized Lagrangian and on Nöther's theory [18]. The matrix approach and the transition to a local coordinate system allows us to formalize and to extend the search for unchanged quantities, which was proposed in [18].

It is rather difficult to compare the equations of motion for the nematic liquid crystal ($q_0 = 0$) in the single-constant approximation of the form (21) and Eqs. (20), (36)–(39) for $K_1 \neq K_2 \neq K_3$, which are written in the original coordinate system, because a large amount of computations is needed. This can be reasonably done by comparing the corresponding functionals for the elastic part of free energy, written in the local coordinate system. In the multi-constant and single-constant cases, the expressions for F_{el}^0 are

$$F_{\text{el}}^0(K_i) = (1/2)[K_1\theta_\xi^2 + K_2\theta_\eta^2 + K_3\theta_\zeta^2 + S_\theta^2(K_2\varphi_\xi^2 + K_1\varphi_\eta^2 + K_3\varphi_\zeta^2)] + S_\theta(K_1 - K_2)(\theta_\xi\varphi_\eta + \theta_\eta\varphi_\xi); \tag{42}$$

$$F_{\text{el}}^0(K) = (K/2)\Big[(\tilde{\nabla}\theta)^2 + S_\theta^2(\tilde{\nabla}\varphi)^2\Big]. \tag{43}$$

We introduce the operators of gradients, in which the spatial variables have different scales, by the expression

$$\tilde{\nabla}_0 = K^{1/2}\Big(\frac{\partial}{\partial\xi}, \frac{\partial}{\partial\eta}, \frac{\partial}{\partial\zeta}\Big), \qquad \tilde{\nabla}_1 = \Big(K_1^{1/2}\frac{\partial}{\partial\xi}, K_2^{1/2}\frac{\partial}{\partial\eta}, K_3^{1/2}\frac{\partial}{\partial\zeta}\Big), \qquad \tilde{\nabla}_2 = \Big(K_2^{1/2}\frac{\partial}{\partial\xi}, K_1^{1/2}\frac{\partial}{\partial\eta}, K_3^{1/2}\frac{\partial}{\partial\zeta}\Big).$$

Then, Eqs. (42) and (43) become

$$F_{\text{el}}^0(K_i) = (1/2)\Big[(\tilde{\nabla}_1\theta)^2 + S_\theta^2(\tilde{\nabla}_2\varphi)^2\Big] + S_\theta(K_1 - K_2)(\theta_\xi\varphi_\eta + \theta_\eta\varphi_\xi); \tag{44}$$

$$F_{\text{el}}^0(K) = (1/2)\Big[(\tilde{\nabla}_0\theta)^2 + S_\theta^2(\tilde{\nabla}_0\varphi)^2\Big]. \tag{45}$$

It follows from a comparison of relations (44) and (45) that the solutions agree qualitatively only if the variation of the last term in (44) is zero or negligibly small. The additive acquires an exact zero value at least in two cases: 1) if the sought solutions depend only on one coordinate variable; 2) if the strained state of the liquid crystal is described by a plane configuration, i.e., one of the angles in the definition of director orientation (4) is identically equal to a constant. The orientation states of liquid crystals considered in the literature mainly refer to these particular cases. In the general form, the solutions of the approximate and exact models are in qualitative agreement if relations of the following form are used in writing the approximate equations:

$$\frac{\delta F_{\rm el}^0}{\delta\theta} = K[\Delta\theta - S_\theta C_\theta(\nabla\varphi)^2] + K_{12}S_\theta\varphi_{xy}, \qquad \frac{\delta F_{\rm el}^0}{\delta\varphi} = K[\mathrm{div}\,(S_\theta^2\nabla\varphi)] + K_{12}S_\theta\theta_{xy} \tag{46}$$

[$\theta_{xy} = \partial^2\theta/\partial x\,\partial y$, $\varphi_{xy} = \partial^2\varphi/\partial x\,\partial y$, $K_{12} \sim (K_1 - K_2)$, and $K \sim (1/3)(K_1 + K_2 + K_3)$ are fitting parameters]. In deriving Eq. (46) in cross components proportional to the difference $K_1 - K_2$, we retained terms that are not repeated in the remaining terms at the coefficients K_i.

Finally, we have to comment on transitions to other coordinate systems. If vector equations of motion written with respect to the director $\boldsymbol{n} = \boldsymbol{n}(t, \boldsymbol{r})$ in the form (3) are used, replacement of variables requires transformations of both coordinates and all vector quantities in the equations. This procedure leads to extremely cumbersome computations, especially in a three-dimensional version. The trigonometric form of recording of the equations of motion (12) with respect to the scalar quantities $\theta = \theta(t, \boldsymbol{r})$ and $\varphi = \varphi(t, \boldsymbol{r})$, as in the transition to a local coordinate system, allows us to transform only the coordinate variables and to leave the sought angles θ and φ defined in the Cartesian coordinate system. An exception is a cylindrical case, because re-definition of the angular variables reduces to simple replacement

$$\theta_{\rm cyl} = \theta_{\rm car}, \qquad \varphi_{\rm cyl} = \varphi_{\rm car} - \alpha,$$

where α is the angular coordinate in a cylindrical coordinate system $\boldsymbol{r} = (\rho, z, \alpha)$. At the same time, re-definition of the functions of the angles in a spherical coordinate system yields nonlinear dependences of the form

$$\cos\theta_{\rm sph} = \cos\theta_{\rm car}\cos\gamma - \sin\theta_{\rm car}\sin\gamma\cos(\varphi_{\rm car} - \alpha), \qquad \varphi_{\rm sph} = \varphi_{\rm car} - \alpha,$$

where γ and α are the angular polar and azimuthal coordinates in a spherical coordinate system $\boldsymbol{r} = (r, \gamma, \alpha)$. The subscripts "cyl," "car," and "sph" mean that the variable is defined in the cylindrical, Cartesian, or spherical coordinate system.

If the sought angular variables are defined in the Cartesian coordinate system, the transition to a new coordinate system is performed by transformation of matrices introduced into the expression for free energy:

$$\tilde{W} = R^{\rm t}WR, \qquad \frac{\partial\tilde{x}_i}{\partial x_j} = R_{ij}.$$

Here $\tilde{x}_i$ are the new coordinates, $R = [R_{ij}]$ is the matrix of the transition $x_i \to \tilde{x}_i$, and W is one of the above-introduced matrices T, Φ, Λ, L, A, and B [see Eqs. (23)–(25), (27), (29), and (30)].

Thus, a matrix approach is proposed for the case of the absence of hydrodynamic flows, and a compact system of equations of orientation motion of the NLC and CLC director in a local coordinate system related to the orientation of the director proper is derived. By analyzing the derived equations, a condition is obtained, which is necessary for qualitative agreement of solutions predicted by the approximate (single-constant) model and those obtained with the exact statement of the problem. A generalized form of the approximate equations is proposed. The matrix form of recording the equations of motion is considered, which allows a fairly simple transition to other coordinate systems and makes it possible to study more sophisticated models for the description of the orientation state of the liquid crystal. The process of derivation of the necessary equations can be readily brought to an algorithm form with the use of symbolic languages. The studies that involve the use of a local coordinate system allow computations for three-dimensional dynamic LC systems even on moderate-performance personal computers. Numerical experiments performed for some particular cases (with the use of the same computational code) showed that the time spend on computations in the local coordinate system can be one tenth of the time needed for integration of equations in the original coordinate system. Test computations showed that solutions predicted by the approximate model (46) are qualitatively identical to results obtained by the exact model, which takes into account the difference in all elastic coefficients.

The author is grateful to S. K. Godunov for consultations and supporting this work.

REFERENCES

1. P. de Genes (ed.), *The Physics of Liquid Crystals*, Clarendon Press, Oxford (1977).
2. S. A. Pikin, *Structural Transformations in Liquid Crystals* [in Russian], Nauka, Moscow (1981).
3. I. P. Suzdalev, *Nanotechnology* [in Russian], KomKniga, Moscow (2005).
4. V. G. Nazarenko, A. B. Nych, and B. I. Lev, "Crystal structure in nematic emulsion," *Phys. Rev. Lett.*, **87**, 075504-1–075504-4 (2001).
5. Jun-ichi-Fukuda, Holger Stark, Makoto Yoneya, and Hiroshi Yokoyama, "Dynamics of a nematic liquid crystal around a spherical particle," *J. Phys. Condens. Matter*, **16**, S1957–S1968 (2004).
6. S. K. Godunov, *Elements of Mechanics of Continuous Media* [in Russian], Nauka, Moscow (1978).
7. S. K. Godunov, *Equations of Mathematical Physics* [in Russian], Nauka, Moscow (1971).
8. S. K. Godunov and T. Yu. Mikhailova, *Presentations of Rotation Groups and Spherical Functions* [in Russian], Nauchnaya Kniga, Novosibirsk (1998).
9. C. W. Oseen, "The theory of liquid crystals," *Trans. Faraday Soc.*, **29**, 883–899 (1933).
10. N. G. Preobrazhenskii and S. I. Trashkeev, "Analytical and numerical methods for computing orientation nonlinearity of liquid crystals," Preprint No. 10-88, Inst. Theor. Appl. Mech., Sib. Div., Acad. of Sci. of the USSR, Novosibirsk (1988).
11. A. S. Zolot'ko, V. F. Kitaeva, N. G. Preobrazhenskii, and S. I. Trashkeev, "On the theory of the Frederix effect in a light field," *Krat. Soobshch. Fiz.*, No. 1, 12–18 (1982).
12. A. S. Zolot'ko, V. F. Kitaeva, N. Kroo, et al., "Numerical calculation of the Frederix threshold in a field of an ordinary-type light wave," *Krat. Soobshch. Fiz.*, No. 10, 30–34 (1984).
13. N. G. Preobrazhenskii and S. I. Trashkeev, "Light-induced Frederix transition in a field of a nonplanar o-wave," *Optika Spektroskop.*, **62**, No. 1, 86–90 (1987).
14. G. M. Zharkova and S. I. Trashkeev, "Orientation of liquid crystals in a spherical volume," *Kristallografiya*, **34**, No. 3, 695–701 (1989).
15. B. Ya. Zel'dovich and N. V. Tabiryan, "Theory of the light-induced Frederix transition," *Zh. Éksp. Teor. Fiz.*, **82**, No. 4, 1126–1146 (1982).
16. J. Nehring and A. Saupe, "On the elastic theory of uniaxial liquid crystals," *J. Chem. Phys.*, **54**, 337–343 (1971).
17. J. Prost and P. S. Pershan, "Flexoelectricity in nematic and smectic-A liquid crystals," *J. Appl. Phys.*, **47**, 2298–2312 (1976).
18. R. S. Akopyan and B. Ya. Zel'dovich, "Laws of conservation and integration of equilibrium equations for liquid crystals," *Zh. Éksp. Teor. Fiz.*, **83**, No. 6, 2137–2145 (1982).