HAMILTONIAN DYNAMICS OF BIAXIAL NEMATICS WITH THE MOLECULAR SHAPE TAKEN INTO ACCOUNT

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We consider the dynamics of biaxial nematics following the Hamiltonian approach. The hydrodynamic parameters related to the broken symmetry are introduced in terms of the distortion tensor. The densities and flows of additive integrals of motion are represented in terms of the thermodynamic potential. We obtain the ideal hydrodynamic equations and study the spectra of collective excitations of biaxial nematics taking the molecular shape into account.

Keywords: Hamiltonian approach, Poisson brackets, biaxial nematics, hydrodynamics, conformational degrees of freedom, acoustic spectra

1. Introduction

In the Hamiltonian approach in the study of the dynamics of condensed media, the structure of the Poisson brackets of the reduced-description parameters plays the fundamental role, completely determining the macroscopic state of the medium. The choice of the parameters of the reduced description in nematic liquid crystals is stipulated by several factors. Some hydrodynamic parameters are related to the symmetry properties of the Hamiltonian, which is manifested in the existence of dynamical equations originating from the differential conservation laws. Another factor affecting the set of hydrodynamic parameters is the molecular shape. In liquid crystals, the molecular shape is related to the structure of the hydrodynamic equations. An additional hydrodynamic quantity in uniaxial nematics is the anisotropy axis determined by the molecular anisotropy [1]. As shown in [2] and [3], the structure of the Poisson brackets of hydrodynamic parameters in such nematics is different for disklike and rodlike molecules. The hydrodynamics of biaxial liquid crystals was studied in [4]. This class of liquid crystals is characterized by a complete spontaneous breaking of the symmetry under rotations in the configuration space $O(3)$. But these papers do not present explicit expressions for all reactive densities of flows of additive integrals of motion in terms of the energy functional and do not explain how the molecular shape affects the dynamical equations for this class of liquid crystals. In addition to these parameters, several scalar parameters related to the molecular shape can arise [5], [6].

Finally, the set of reduced-description parameters is related to the character of spontaneous symmetry breaking in the system. The statement of elasticity theory as a division of continuum mechanics is based on the idea that the translational symmetry can be broken spontaneously. An additional macroscopic quantity, the deformation tensor, is introduced as a function of the distortion tensor [7]. This quantity completely characterizes the character of continuum deformation. The hydrodynamic theory of liquid crystals is also a division of continuum mechanics in which the symmetry under rotations (and under translations in some

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cases) in the configuration space is broken spontaneously. It was shown in [3] and [5] that the additional hydrodynamic parameters related to this symmetry breaking can be represented in terms of the distortion tensor for several uniaxial and biaxial liquid crystals.

In this paper, we introduce the additional quantities related to any spontaneous breaking of the symmetry under rotations in the configuration space in terms of the distortion tensor, represent the densities and flows of additive integrals of motion in terms of the thermodynamic potential, obtain the ideal hydrodynamic equations, and study the spectra of collective excitations of biaxial liquid crystals taking the molecular shape into account.

2. Poisson brackets in the dynamical theory of liquid crystals

In the Hamiltonian approach, the equations of motion for the reduced-description parameters can be written as

$$\dot{\varphi}_\alpha(x) = \big\{\varphi_\alpha(x), H(\varphi)\big\}, \tag{2.1}$$

where $H(\varphi)$ is the Hamiltonian of the system. The Poisson bracket of arbitrary functionals is determined by the relation

$$\{A, B\} \equiv \int d^3x \int d^3x' \, \frac{\delta A}{\delta\varphi_\alpha(x)} \big\{\varphi_\alpha(x), \varphi_\beta(x')\big\} \frac{\delta B}{\delta\varphi_\beta(x')}, \tag{2.2}$$

where the Poisson brackets of the quantities $\varphi_\alpha(x)$ are antisymmetric under permutations and satisfy the Jacobi identity. The relations

$$\{A, B\} = -\{B, A\}, \qquad \{AB, C\} = A\{B, C\} + B\{A, C\},$$
$$\big\{A, \{B, C\}\big\} + \big\{B, \{C, A\}\big\} + \big\{C, \{A, B\}\big\} = 0$$

therefore hold for arbitrary functionals.

The conservation laws can be written in differential form as

$$\dot{\zeta}_a(x) = -\nabla_k \zeta_{ak}(x), \tag{2.3}$$

where $\zeta_a(x)$ are the functions $\varepsilon(x)$, $\pi_k(x)$, or $\rho(x)$, i.e., the densities of additive integrals of motion ($\varepsilon(x)$ is the energy density, $a = 0$; $\pi_k(x)$ is the density of the kth momentum component, $a = k$; and $\rho(x)$ is the mass density, $a = 4$) and $\zeta_{ak}(x)$ are the functions $q_k(x)$, $t_{ik}(x)$, or $j_k(x)$, i.e., the corresponding densities of flows of additive integrals of motion. As shown in [8], the following representation of densities of flows of additive integrals of motion holds in terms of the Poisson brackets of the corresponding densities $\zeta_a(x)$:

$$\zeta_{ak}(x) = -\delta_{ak}\varepsilon(x) + \int d^3x' \, x'_k \int_0^1 d\lambda \, \big\{\zeta_a(y), \varepsilon(y')\big\}, \quad a \neq 0, \tag{2.4}$$
$$\zeta_{0k}(x) = \frac{1}{2}\int d^3x' \, x'_k \int_0^1 d\lambda \, \big\{\varepsilon(y), \varepsilon(y')\big\},$$
$$y \equiv x + \lambda x', \qquad y' \equiv x - (1-\lambda)x'.$$

We consider the distortion tensor

$$b_{ki}(x) \equiv \delta_{ki} - \nabla_i u_k(x), \tag{2.5}$$

which is determined via the displacement vector $u_k(x)$ relating the Lagrangian coordinate ξ_k to the Euler coordinate $x_k = \xi_k + u_k(x)$. The distortion tensor $b_{ki}(x)$ given by (2.5) determines the orientational and translational states of an arbitrary continuous medium. The true density $\rho(x)$ of the matter in an arbitrary state is determined in terms of the distortion tensor by the relation [3],

$$\rho(x) = \underline{\rho}\, \det\bigl|b_{ij}(x)\bigr|, \tag{2.6}$$

where $\underline{\rho}$ is the density of the matter in the nondeformed state. The Poisson brackets of the momentum densities, the mass density, the entropy density $\sigma(x)$, and the distortion tensor can be written as [3]

$$\begin{aligned}
&\bigl\{\pi_i(x), \sigma(x')\bigr\} = -\sigma(x)\nabla_i \delta(x - x'), \qquad \bigl\{\pi_i(x), b_{kj}(x')\bigr\} = -b_{ki}(x)\nabla_j \delta(x - x'),\\
&\bigl\{\pi_i(x), \pi_j(x')\bigr\} = \pi_j(x)\nabla'_i \delta(x - x') - \pi_i(x')\nabla_j \delta(x - x'),\\
&\bigl\{\pi_i(x), \rho(x')\bigr\} = \rho(x)\nabla'_i \delta(x - x').
\end{aligned} \tag{2.7}$$

These Poisson brackets underlie the construction of nonlinear hydrodynamic-type equations for normal liquids, crystals, and liquid crystals. The influence of the molecular shape in liquid crystals on the dynamical properties is manifested in different forms of the dependence of energy on the distortion tensor. In what follows, considering specific examples, we show how the form of the reduced-description parameters can be chosen depending on the molecular shape. We next take into account that the Hamiltonian of the system has the Galilei-invariant form

$$H = \int d^3x \left(\frac{\pi_i^2(x)}{2\rho(x)} + \Phi\bigl(\rho(x), \sigma(x), b_{ij}(x)\bigr) \right). \tag{2.8}$$

In this case, we have $m j_k(x) = \pi_k(x)$, where m is the particle mass.

3. Dynamics of biaxial nematics with disklike molecules

We consider condensed media with a spontaneously broken symmetry under rotations in the configuration space. Liquid crystals belong to this class of condensed media. First, we note that the state of an isotropic liquid is described by dynamical variables such as the mass, momentum, and entropy densities. To have these macroscopic parameters is insufficient for describing the nematic phase of liquid crystals because a spontaneous breaking of the rotational symmetry due to the anisotropy of molecules can occur in this state. In [4], two anisotropy axes representing the anisotropy property of molecules were introduced as additional reduced-description parameters in the case of biaxial nematics. Because the molecules have a complicated shape, a larger number of parameters is required for their macroscopic description. Additional macroscopic parameters for uniaxial liquid crystals are the molecular length in the case of rodlike molecules and the disk area in the case of disklike molecules. The molecular shape in biaxial liquid crystals can be determined by the lengths of the major and minor anisotropy axes and the angle between them. In what follows, the parameters used to describe the molecular shape are called the *conformational degrees of freedom*. This extension of the set of reduced-description parameters for liquid crystals is due to the anisotropy properties and the conformational nonrigidity of molecules [5], [6]. We begin our study of biaxial liquid crystals with the case of disklike molecules. Let $\vec{m}(x)$ and $\vec{n}(x)$ be the unit orthogonal vectors determining the anisotropy axes and characterizing the breaking of rotational invariance by the relations

$$n_i(x) \equiv \frac{a(x)b_i(x) + b(x)a_i(x)}{\bigl|a(x)\vec{b}(x) + b(x)\vec{a}(x)\bigr|}, \qquad m_i(x) \equiv \frac{a(x)b_i(x) - b(x)a_i(x)}{\bigl|a(x)\vec{b}(x) - b(x)\vec{a}(x)\bigr|}, \tag{3.1}$$

where the vectors $\vec{a}(x)$ and $\vec{b}(x)$ are represented in terms of the distortion tensor,

$$a_j(x) \equiv e_{1k} b_{kj}(x), \qquad b_j(x) \equiv e_{2k} b_{kj}(x). \tag{3.2}$$

The constant vectors $\vec{e}_1$ and $\vec{e}_2$ determine the directions of the anisotropy axes and the dimensions of disklike molecules in a nondeformed liquid crystal. Any deformation of the medium results in changes in the directions of the anisotropy axes and in the molecular dimensions, and these changes are described by the distortion tensor. According to formulas (2.7), (3.1), and (3.2), we obtain the Poisson brackets of the momentum density $\pi_k(x)$ and the unit vectors $n_k(x)$ and $m_k(x)$:

$$\begin{aligned} \big\{\pi_i(x), n_j(x')\big\} &= \delta(x-x')\nabla_i n_j(x) + f_{i\lambda j}(x')\nabla'_\lambda \delta(x-x'), \\ \big\{\pi_i(x), m_j(x')\big\} &= \delta(x-x')\nabla_i m_j(x) + g_{i\lambda j}(x')\nabla'_\lambda \delta(x-x'), \end{aligned} \tag{3.3}$$

where the functions $f_{i\lambda j}(x)$ and $g_{i\lambda j}(x)$ are determined by the relations

$$\begin{aligned} f_{i\lambda j}(x) &\equiv n_i(x)\delta^{\perp}_{j\lambda}\big(\vec{n}(x)\big) - p(x)m_j(x)\big(n_i(x)m_\lambda(x) + n_\lambda(x)m_i(x)\big), \\ g_{i\lambda j}(x) &\equiv m_i(x)\delta^{\perp}_{j\lambda}\big(\vec{m}(x)\big) - \big(1-p(x)\big)n_j(x)\big(n_i(x)m_\lambda(x) + n_\lambda(x)m_i(x)\big), \\ \delta^{\perp}_{kj}\big(f(x)\big) &\equiv \delta_{kj} - f_k(x)f_j(x). \end{aligned} \tag{3.4}$$

The quantity

$$p(x) \equiv \frac{1}{2}\left(1 - \frac{\vec{a}(x)\vec{b}(x)}{a(x)b(x)}\right) \tag{3.5}$$

determines the angle between the anisotropy axes in a deformed state. We see that to close the Poisson bracket algebra of the hydrodynamic parameters for these liquid crystals, it is insufficient to introduce only the anisotropy axes. It is necessary to extend the set of reduced-description parameters because the right-hand sides of relations (3.3) contain the quantity $p(x)$. The Poisson bracket of this quantity and the momentum density has the form

$$\begin{aligned} \big\{\pi_i(x), p(x')\big\} &= \delta(x-x')\nabla_i p(x) + h_{il}(x')\nabla'_l \delta(x-x'), \\ h_{ik} &\equiv 2p(1-p)(m_i m_k - n_i n_k). \end{aligned} \tag{3.6}$$

According to (2.7), (3.3), and (3.6), the Poisson brackets for the set of reduced-description parameters $\sigma(x)$, $\pi_k(x)$, $\rho(x)$, $\vec{m}(x)$, $\vec{n}(x)$, and $p(x)$ form a subalgebra of Poisson bracket algebra (2.7) of the dynamical continuum variables. For biaxial liquid crystals, in addition to the quantity $p(x)$, it is generally possible to introduce two more conformational degrees of freedom representable in terms of the distortion tensor as

$$\bar{a}(x) \equiv 2\big|\vec{a}(x)\big|\big(1-p(x)\big)^{1/2}, \qquad \bar{b}(x) \equiv 2\big|\vec{b}(x)\big|p^{1/2}(x). \tag{3.7}$$

These quantities, together with (3.5), determine the dimensions and the molecular shape in liquid crystals in a deformed state.

From definitions (3.7) with (3.2) and (2.7) taken into account, we obtain the Poisson brackets of the conformational degrees of freedom and the momentum density

$$\begin{aligned} \{\pi_i(x),\bar{a}(x')\} &= \delta(x-x')\nabla_i\bar{a}(x)+f_{ij}(x')\nabla'_j\delta(x-x'),\\ \{\pi_i(x),\bar{b}(x')\} &= \delta(x-x')\nabla_i\bar{b}(x)+g_{ij}(x')\nabla'_j\delta(x-x'), \end{aligned} \tag{3.8}$$

where we use the notation

$$\begin{aligned} f_{ik} &= \bar{a}\big(n_i n_k - \sqrt{p(1-p)}\,(n_i m_k + n_k m_i)\big),\\ g_{ik} &= \bar{b}\big(m_i m_k + \sqrt{p(1-p)}\,(n_i m_k + n_k m_i)\big). \end{aligned}$$

The orientational $\vec{m}(x)$, $\vec{n}(x)$ and conformational $\bar{a}(x)$, $\bar{b}(x)$, $p(x)$ degrees of freedom are local functions of the distortion tensor and are treated as independent variables. The set of reduced-description parameters consists of the densities of additive integrals of motion, the two vectors $n_k(x)$ and $m_k(x)$ characterizing the anisotropy axes, and the three conformational parameters: $\varphi_\alpha(x)\equiv\{\varsigma_a(x),\vec{n}(x),\vec{m}(x),\bar{a}(x),\bar{b}(x),p(x)\}$. In uniaxial nematics, the set of parameters decreases and becomes $\varphi_\alpha(x)\equiv\{\varsigma_a(x),\vec{n}(x),\bar{a}(x)\}$. Poisson brackets (2.7), (3.3), (3.6), and (3.8) form a closed algebra of hydrodynamic variables of a biaxial nematic with disklike molecules; in this case, the density of the condensed medium energy is a function of these variables,

$$\varepsilon(x)=\varepsilon\big(\sigma(x),\vec{\pi}(x),\rho(x),\vec{n}(x),\nabla\vec{n}(x),\vec{m}(x),\nabla\vec{m}(x),\bar{a}(x),\bar{b}(x),p\big). \tag{3.9}$$

We introduce the thermodynamic potential density

$$\omega\equiv\frac{\partial\sigma}{\partial\varsigma_a}\zeta_a-\sigma.$$

Then the second law of thermodynamics can be written as

$$\begin{aligned} d\omega &= \varepsilon\,dY_0+\pi_i\,dY_i+\rho\,dY_4+\left(\frac{\partial\omega}{\partial n_i}-\nabla_j\frac{\partial\omega}{\partial\nabla_j n_i}\right)dn_i+\frac{\partial\omega}{\partial p}\,dp+\frac{\partial\omega}{\partial\bar{a}}\,d\bar{a}+\frac{\partial\omega}{\partial\bar{b}}\,d\bar{b}+\\ &+\left(\frac{\partial\omega}{\partial m_i}-\nabla_j\frac{\partial\omega}{\partial\nabla_j m_i}\right)dm_i+\nabla_j\left(\frac{\partial\omega}{\partial\nabla_j n_i}\,dn_i+\frac{\partial\omega}{\partial\nabla_j m_i}\,dm_i\right), \end{aligned} \tag{3.10}$$

where $Y_0^{-1}=T$ is the temperature, $-Y_k/Y_0=v_k$ is the velocity, and $-Y_4/Y_0=\mu$ is the chemical potential. Taking Poisson brackets (2.7), (3.3), (3.6), and (3.8) and formula (2.4) into account, we obtain the hydrodynamic equations for the biaxial phase of a nematic with disklike molecules from equations of motion (2.1) in Hamiltonian form:

$$\begin{aligned} &\dot{\sigma}(x)=-\nabla_i\big(\sigma(x)\nu_i(x)\big),\qquad \dot{\rho}(x)=-\nabla_i\pi_i(x),\qquad \dot{\pi}_i(x)=-\nabla_k t_{ik}(x),\\ &\dot{n}_j(x)=-\nu_s(x)\nabla_s n_j(x)-f_{i\lambda j}(x)\nabla_\lambda\nu_i(x),\\ &\dot{m}_j(x)=-\nu_s(x)\nabla_s m_j(x)-g_{i\lambda j}(x)\nabla_\lambda\nu_i(x),\\ &\dot{p}(x)=-\nu_s(x)\nabla_s p(x)-h_{kl}(x)\nabla_k\nu_l(x),\\ &\dot{\bar{a}}(x)=-\nu_i(x)\nabla_i\bar{a}(x)-f_{ij}(x)\nabla_j\nu_i(x),\\ &\dot{\bar{b}}(x)=-\nu_i(x)\nabla_i\bar{b}(x)-g_{ij}(x)\nabla_j\nu_i(x). \end{aligned} \tag{3.11}$$

The momentum flux density $t_{ik}(x)$ can be found by using the set of Poisson brackets (2.7), (3.3), (3.6), and (3.8) and formula (2.4) and can be written in terms of the thermodynamic potential density:

$$
\begin{aligned}
t_{ik} &= t^0_{ik} + t'_{ik}, \qquad t^0_{ik} = -\frac{\partial}{\partial Y_i}\frac{\omega Y_k}{Y_0},\\
t'_{ik} &= \frac{1}{Y_0}\left[\frac{\partial\omega}{\partial\nabla_k n_j}\nabla_i n_j + \frac{\partial\omega}{\partial\nabla_k m_j}\nabla_i m_j + f_{ikl}\left(\frac{\partial\omega}{\partial n_l} - \nabla_j\frac{\partial\omega}{\partial\nabla_j n_l}\right) + \right.\\
&\left. + g_{ikl}\left(\frac{\partial\omega}{\partial m_l} - \nabla_j\frac{\partial\omega}{\partial\nabla_j m_l}\right) + \frac{\partial\omega}{\partial p}h_{ik} + \frac{\partial\omega}{\partial\bar a}f_{ik}\bar a + \frac{\partial\omega}{\partial\bar b}g_{ik}\bar b\right].
\end{aligned}
\tag{3.12}
$$

Formulas (3.10)–(3.12) give a complete set of ideal hydrodynamic equations for a biaxial nematic consisting of disklike molecules with three conformational degrees of freedom.

We use the obtained equations of biaxial nematics to study the spectra of collective excitations. We assume that the equilibrium of the medium is homogeneous and nondeformed ($p = 1/2$) and the medium as a whole is at rest ($\nu_k = 0$). This means that

$$
\begin{aligned}
\frac{\partial\omega}{\partial n_k} &= \frac{\partial\omega}{\partial\nabla_l n_k} = \frac{\partial^2\omega}{\partial n_k\partial\nabla_l n_j} = 0,\\
\frac{\partial\omega}{\partial m_k} &= \frac{\partial\omega}{\partial\nabla_l m_k} = \frac{\partial^2\omega}{\partial m_k\partial\nabla_l m_j} = 0,\\
\frac{\partial\omega}{\partial v_k} &= \frac{\partial^2\omega}{\partial v_j\partial n_k} = \frac{\partial^2\omega}{\partial v_k\partial\nabla_l n_j} = 0.
\end{aligned}
$$

Linearizing system of equations (3.10)–(3.12), we obtain the equations for small deviations of the parameters of a biaxial nematic from equilibrium:

$$
\begin{aligned}
\delta\dot\rho &= -\rho\nabla_j v_j, \qquad \delta\dot s = 0, \qquad \delta\dot p = \frac{1}{2}(n_i n_l - m_i m_l)\nabla_i v_l,\\
\rho\delta\dot v_i &= \frac{\partial\mathcal{P}}{\partial\rho}\nabla_i\rho + \frac{1}{2Y_0}(n_i n_l - m_i m_l)\left[\frac{\partial^2\omega}{\partial p^2}\nabla_l\delta p + \frac{\partial^2\omega}{\partial p\partial n}\nabla_l\delta n\right],\\
\delta\dot n_j &= \left[-n_l\delta^{\perp}_{\lambda j}(\vec n) + \frac{1}{2}(n_\lambda m_l + n_l m_\lambda)\right]\nabla_\lambda\delta v_l,\\
\delta\dot m_j &= \left[-m_l\delta^{\perp}_{\lambda j}(\vec m) + \frac{1}{2}(n_\lambda m_l + n_l m_\lambda)\right]\nabla_\lambda\delta v_l,
\end{aligned}
\tag{3.13}
$$

where $s \equiv \sigma/n$, n is the particle density, and $\mathcal{P} \equiv -\omega/Y_0$ is the pressure. Deriving system of equations (3.13), we take into account that according to (3.5), the minimum is realized at the point $p = 1/2$ in the nondeformed state, i.e., $(\partial\omega/\partial p)\big|_{p=1/2} = 0$. We assume that the term $\partial^2\omega/(\partial p\,\partial n)$ is small compared with $\partial^2\omega/\partial p^2$. We also assume that solutions of Eqs. (3.13) contain the space–time dependence $e^{i(\Omega t - \vec k\vec x)}$. As a result, we obtain the dispersion equation for the spectra of collective excitations

$$
\begin{aligned}
&\det\left(\Omega^2\delta_{ij} - k_i k_j\frac{\partial\mathcal{P}}{\partial\rho} - D_{imjl}k_m k_l\right) = 0,\\
&D_{imjl} = A f_{im}f_{jl} + B g_{im}g_{jl} + C h_{im}h_{jl},\\
&A \equiv \frac{1}{Y_0\rho}\frac{\partial^2\omega}{\partial a^2}, \qquad B \equiv \frac{1}{Y_0\rho}\frac{\partial^2\omega}{\partial b^2}, \qquad C \equiv \frac{1}{Y_0\rho}\frac{\partial^2\omega}{\partial p^2}.
\end{aligned}
\tag{3.14}
$$

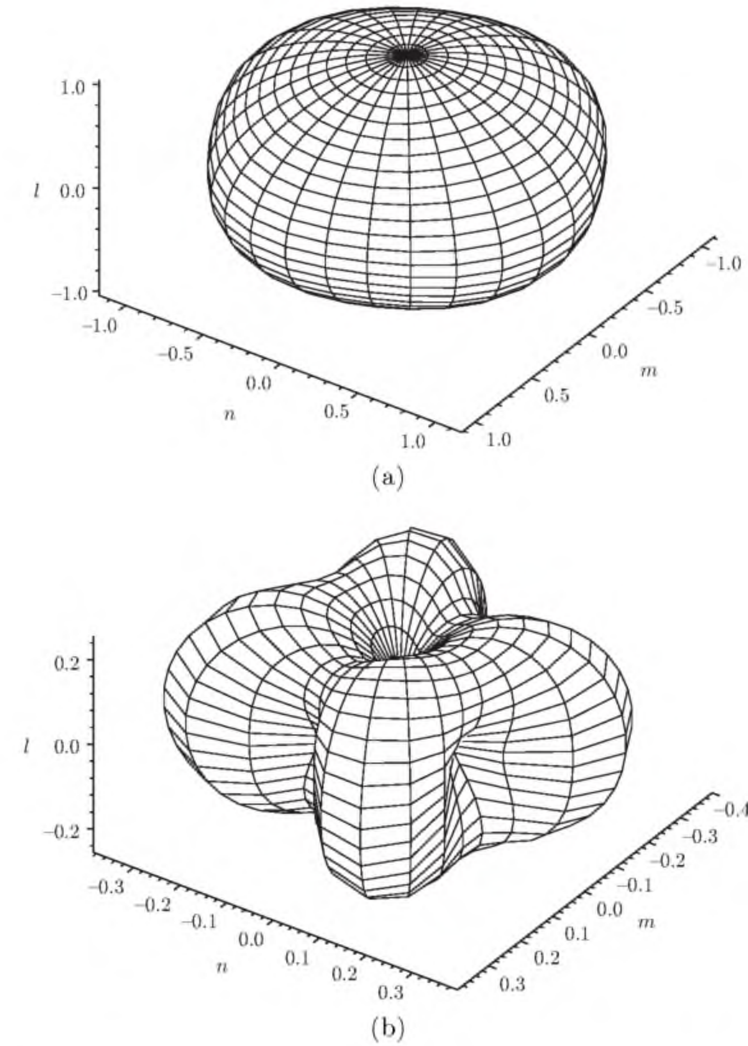

Fig. 1. Angle dependence of the velocities $c_+(\theta,\varphi)$ (a) and $c_-(\theta,\varphi)$ (b) for the parameter values $\lambda_a = 0.1$, $\lambda_b = 0.2$, and $\lambda_c = 0.05$.

Calculating the determinant, we obtain the equation

$$\Omega^2\big(\Omega^4 - \Omega^2 L_4(\vec{k}) + L_2(\vec{k})\big) = 0, \tag{3.15}$$

where we use the notation

$$\begin{aligned}
L_4(\vec{k}) &= k^2c^2\big[1 + \Phi(\varphi,\lambda)\sin^2\theta\big],\\
L_2(\vec{k}) &= k^4c^4\bigg\{\Phi(\varphi,\lambda)\sin^2\theta\cos^2\theta + \frac{1}{2}(\lambda_a+\lambda_b)\sin^4\theta\sin^2\left(\frac{\pi}{4}+2\varphi\right) +\\
&\quad + \sin^4\theta\bigg[\lambda_c\sin^2 2\varphi + \frac{1}{2}\lambda_a\lambda_b\sin^2\left(\frac{\pi}{4}+2\varphi\right) +\\
&\quad + \lambda_a\lambda_c\sin^4\left(\frac{\pi}{4}-\varphi\right) + \lambda_c\lambda_b\sin^4\left(\frac{\pi}{4}+\varphi\right)\bigg]\bigg\},\\
\Phi(\varphi,\lambda) &\equiv \frac{3}{4}(\lambda_a+\lambda_b) + \frac{1}{\sqrt{2}}(\lambda_a-\lambda_b)\sin\left(\frac{\pi}{4}-2\varphi\right) + \lambda_c,
\end{aligned} \tag{3.16}$$

where $c^2 = \partial\mathcal{P}/\partial\rho$ is the velocity of sound in the isotropic state of the condensed medium under study $\lambda_a \equiv a^2A/c^2$, $\lambda_b \equiv b^2B/c^2$, and $\lambda_c \equiv C/(4c^2)$. We introduce the polar and azimuth angles θ and φ determining the direction of the wave vector $\vec{e} \equiv \vec{k}/k$: $\vec{e}\vec{m} = \sin\theta\cos\varphi$, $\vec{e}\vec{n} = \sin\theta\sin\varphi$, and $\vec{e}\vec{l} = \cos\theta$. We see that two branches of acoustic oscillations corresponding to the first and second sounds can propagate in a biaxial nematic with disklike molecules:

$$\Omega^2_\pm(\vec{k}) = \frac{1}{2}\left(L_4(\vec{k}) \pm \sqrt{L_4^2(\vec{k}) - 4L_2(\vec{k})}\right) \equiv k^2 c^2_\pm(\vec{e}), \tag{3.17}$$

where the solution with the plus sign determines a sound similar to that in a normal liquid and the solution with the minus sign determines the second sound, i.e., a new branch of excitations due to the conformational degrees of freedom of the biaxial liquid crystal.

The anisotropy of the velocities of sounds is essential for both solutions. It follows from (3.16) and (3.17) that

$$\begin{gathered} c_\pm(\theta,\varphi) = \frac{c}{\sqrt{2}}\Big\{1 + \Phi(\varphi,\lambda)\sin^2\theta \pm \big[\big(1 - \Phi(\varphi,\lambda)\sin^2\theta\big)^2 + 4Q(\varphi,\lambda)\sin^4\theta\big]^{1/2}\Big\}^{1/2}, \\ Q(\varphi,\lambda) \equiv \Phi(\varphi,\lambda) - \frac{1}{2}(\lambda_a + \lambda_b + \lambda_a\lambda_b)\sin^2\left(\frac{\pi}{4} + 2\varphi\right) - \\ - \lambda_a\lambda_c\sin^4\left(\frac{\pi}{4} - \varphi\right) - \lambda_c\lambda_b\sin^4\left(\frac{\pi}{4} + \varphi\right) - \lambda_c\sin^2 2\varphi. \end{gathered} \tag{3.18}$$

Figure 1 demonstrates the character of anisotropy (3.18) (the three vectors $\vec{m}$, $\vec{n}$, and $\vec{l}$ form the rectangular Cartesian coordinate system).

Comparing formulas (3.18) with the results in [4], we see that the reactive component in the spectrum of the second sound can already be obtained in the adiabatic approximation if the conformational degrees of freedom are taken into account in the hydrodynamic equations of a biaxial nematic.

4. Dynamics of biaxial nematics with rodlike molecules

In the case of rodlike molecules, the unit orthogonal anisotropy axes $\vec{m}(x)$ and $\vec{n}(x)$ characterizing the breaking of rotational invariance are determined by the relations

$$n_i(x) = \frac{A(x)B_i(x) + B(x)A_i(x)}{\big|A(x)\vec{B}(x) + B(x)\vec{A}(x)\big|}, \qquad m_i(x) = \frac{A(x)B_i(x) - B(x)A_i(x)}{\big|A(x)\vec{B}(x) - B(x)\vec{A}(x)\big|}. \tag{4.1}$$

The vectors

$$A_j(x) \equiv e_{1k}b^{-1}_{kj}(x), \qquad B_j(x) \equiv e_{2k}b^{-1}_{kj}(x) \tag{4.2}$$

are given here in terms of the inverse matrix $b^{-1}_{kj}(x)$. Because the inverse matrix has the form

$$(b^{-1})_{c'c} = \frac{1}{2\det b}\varepsilon_{abc}\varepsilon_{a'b'c'}b_{aa'}b_{bb'}, \qquad \det b = \frac{1}{6}\varepsilon_{abc}\varepsilon_{a'b'c'}b_{aa'}b_{bb'}b_{cc'}, \tag{4.3}$$

according to this formula, definitions (4.1), and relations (2.7), we obtain the Poisson brackets of the vectors $\vec{m}(x)$ and $\vec{n}(x)$ and the momentum density

$$\begin{aligned} \big\{\pi_i(x), n_j(x')\big\} &= \delta(x - x')\nabla_i n_j(x) + F_{i\lambda j}(x')\nabla'_\lambda\delta(x - x'), \\ \big\{\pi_i(x), m_j(x')\big\} &= \delta(x - x')\nabla_i m_j(x) + G_{i\lambda j}(x')\nabla'_\lambda\delta(x - x'), \end{aligned} \tag{4.4}$$

where we use the notation

$$F_{i\lambda j}(x) \equiv -n_\lambda(x)\delta^{\perp}_{ij}\big(\vec{n}(x)\big) + P(x)m_j(x)\big(n_i(x)m_\lambda(x) + n_\lambda(x)m_i(x)\big),$$
$$G_{i\lambda j}(x) \equiv -m_\lambda(x)\delta^{\perp}_{ij}\big(\vec{m}(x)\big) + \big(1 - P(x)\big)N_j(x)\big(n_i(x)m_\lambda(x) + n_\lambda(x)m_i(x)\big).$$

The shape factor

$$P(x) \equiv \frac{1}{2}\left(1 - \frac{\vec{A}(x)\vec{B}(x)}{A(x)B(x)}\right) \tag{4.5}$$

and the conformational parameters

$$\overline{A}(x) \equiv 2\big|\vec{A}(x)\big|\big(1 - P(x)\big)^{1/2}, \qquad \overline{B}(x) \equiv 2\big|\vec{B}(x)\big|P^{1/2}(x) \tag{4.6}$$

are introduced to take the shape and dimensions of rodlike molecules into account. It follows from definitions (4.5) and (4.6) and formulas (2.7) that

$$\begin{aligned}
\big\{\pi_i(x), P(x')\big\} &= \delta(x - x')\nabla_i P(x) + 2H_{ij}(x')\nabla'_j\delta(x - x'),\\
\big\{\pi_i(x), \overline{A}(x')\big\} &= \delta(x - x')\nabla_i \overline{A}(x) + F_{ij}(x')\nabla'_j\delta(x - x'),\\
\big\{\pi_i(x), \overline{B}(x')\big\} &= \delta(x - x')\nabla_i \overline{B}(x) + G_{ij}(x')\nabla'_j\delta(x - x'),
\end{aligned} \tag{4.7}$$

where we set

$$\begin{aligned}
F_{ik} &= \overline{A}\big(\delta^{\perp}_{ik}(\vec{n}) - \sqrt{P(1-P)}\,(n_i m_k + n_k m_i)\big),\\
G_{ik} &= \overline{B}\big(\delta^{\perp}_{ik}(\vec{m}) + \sqrt{P(1-P)}\,(n_i m_k + n_k m_i)\big),\\
H_{ik} &= -2P(1-P)(m_i m_k - n_i n_k).
\end{aligned} \tag{4.8}$$

Expressions (2.4), (2.7), (4.4), and (4.7) permit finding the densities of flows of additive integrals of motion in terms of the thermodynamic potential:

$$\begin{aligned}
\zeta_{ak} &= \zeta^0_{ak} + \zeta'_{ak}, \qquad \zeta^0_{ak} = -\frac{\partial}{\partial Y_a}\frac{\omega Y_k}{Y_0},\\
\zeta'_{ak} &= \left[\frac{\partial\omega}{\partial\nabla_k n_j}\nabla_i n_j + \frac{\partial\omega}{\partial\nabla_k m_j}\nabla_i m_j + F_{ikl}\left(\frac{\partial\omega}{\partial n_l} - \nabla_j\frac{\partial\omega}{\partial\nabla_j n_l}\right) + \right.\\
&\quad \left. + G_{ikl}\left(\frac{\partial\omega}{\partial m_l} - \nabla_j\frac{\partial\omega}{\partial\nabla_j m_l}\right) + H_{ik}\frac{\partial\omega}{\partial P} + \frac{\partial\omega}{\partial\overline{A}}F_{ik} + \frac{\partial\omega}{\partial\overline{B}}G_{ik}\right]\frac{\partial}{\partial Y_a}\frac{Y_i}{Y_0}.
\end{aligned} \tag{4.9}$$

The set of reduced-description parameters consists of the densities of additive integrals of motion, the two vectors $\vec{m}(x)$ and $\vec{n}(x)$, and the three conformational parameters: $\varphi_\alpha(x) \equiv \big\{\varsigma_a(x), \vec{m}(x), \vec{m}(x), \bar{A}(x), \overline{B}(x), P(x)\big\}$. This set forms a closed Poisson bracket algebra.

Next, proceeding as in the case of disklike molecules, we easily derive the local ideal hydrodynamic equations for biaxial nematics with rodlike molecules with three conformational degrees of freedom:

$$\begin{aligned}
&\dot{\sigma}(x) = -\nabla_i\big(\sigma(x)\nu_i(x)\big), \qquad \dot{\rho}(x) = -\nabla_i \pi_i(x), \qquad \dot{\pi}_i(x) = -\nabla_k t_{ik}(x),\\
&\dot{n}_j(x) = -\nu_s(x)\nabla_s n_j(x) - F_{i\lambda j}(x)\nabla_\lambda \nu_i(x),\\
&\dot{m}_j(x) = -\nu_s(x)\nabla_s m_j(x) - G_{i\lambda j}(x)\nabla_\lambda \nu_i(x),\\
&\dot{\overline{A}}(x) = -\nu_i(x)\nabla_i \overline{A}(x) - F_{ij}(x)\nabla_j \nu_i(x),\\
&\dot{\overline{B}}(x) = -\nu_i(x)\nabla_i \overline{B}(x) - G_{ij}(x)\nabla_j \nu_i(x),\\
&\dot{P}(x) = -\nu_i(x)\nabla_i P(x) - H_{ij}(x)\nabla_j \nu_i(x).
\end{aligned} \tag{4.10}$$

We linearize these equations and seek their solution in the form $\sim e^{i(\Omega t - \vec{k}\vec{x})}$. Linearizing the equations leads to the bicubic dispersion equation

$$\Omega^6 + I_4(\theta,\varphi)\Omega^4 + I_2(\theta,\varphi)\Omega^2 + I_0(\theta,\varphi) = 0, \tag{4.11}$$

where the coefficients $I_4(\theta,\varphi)$, $I_2(\theta,\varphi)$, and $I_0(\theta,\varphi)$ have the forms

$$\begin{aligned}
I_4(\theta,\varphi) =& -k^2c^2\left\{1 + \sin^2\theta\left[(\lambda_1+\lambda_2)\left(\cot^2\theta + \frac{3}{4}\right) - \frac{1}{\sqrt{2}}\left(\lambda_1-\lambda_2\right)\sin\left(\frac{\pi}{4} - 2\varphi\right) + \lambda_3\right]\right\},\\
I_2(\theta,\varphi) =& \, k^2c^2\big(I_4(\theta,\varphi) + k^2c^2\big) +\\
&+ k^4c^4\sin^4\theta\left\{\lambda_1\lambda_2\left[2\cot^2\theta + \frac{1}{2}\sin^2\left(\frac{\pi}{4} + 4\varphi\right)\right] +\right.\\
&+ \lambda_1\lambda_3\left[\cot^2\theta + \sin^4\left(\frac{\pi}{4} + 2\varphi\right)\right] +\\
&+ \lambda_2\lambda_3\left[\cot^2\theta + \sin^4\left(\frac{\pi}{4} - 2\varphi\right)\right] - \lambda_3\cos^2 2\varphi - (\lambda_1+\lambda_2)\times\\
&\times\left[\cot^4\theta + \cot^2\theta - \frac{1}{2}\sin^2\left(\frac{\pi}{4} + 4\varphi\right) + \frac{3}{4}\right] +\\
&\left.+ \frac{1}{\sqrt{2}}(\lambda_1-\lambda_2)\left[\cot^2\theta + \frac{1}{2}\right]\sin\left(\frac{\pi}{4} - 2\varphi\right)\right\},\\
I_0(\theta,\varphi) =& -k^6c^6\lambda_1\lambda_2\lambda_3\sin^4\theta\cos^2\theta.
\end{aligned}$$

Here, we introduce the dimensionless quantities

$$\lambda_1 \equiv \frac{\bar{A}^2}{\rho Y_0 c^2}\frac{\partial^2\omega^2}{\partial\bar{A}^2}, \qquad \lambda_2 \equiv \frac{\overline{B}^2}{\rho Y_0 c^2}\frac{\partial^2\omega}{\partial\overline{B}^2}, \qquad \lambda_3 \equiv \frac{1}{4\rho Y_0 c^2}\frac{\partial^2\omega}{\partial P^2}.$$

An analysis of Eq. (4.11) (cubic with respect to Ω^2) shows that in the range of the parameters λ_i where the determinant of the equation is negative, the condensed medium under study is characterized by three acoustic spectra. We introduce the notation $y = \Omega^2 + I_4/3$ and transform Eq. (4.11) to the reduced form

$$y^3 + qy + t = 0,$$

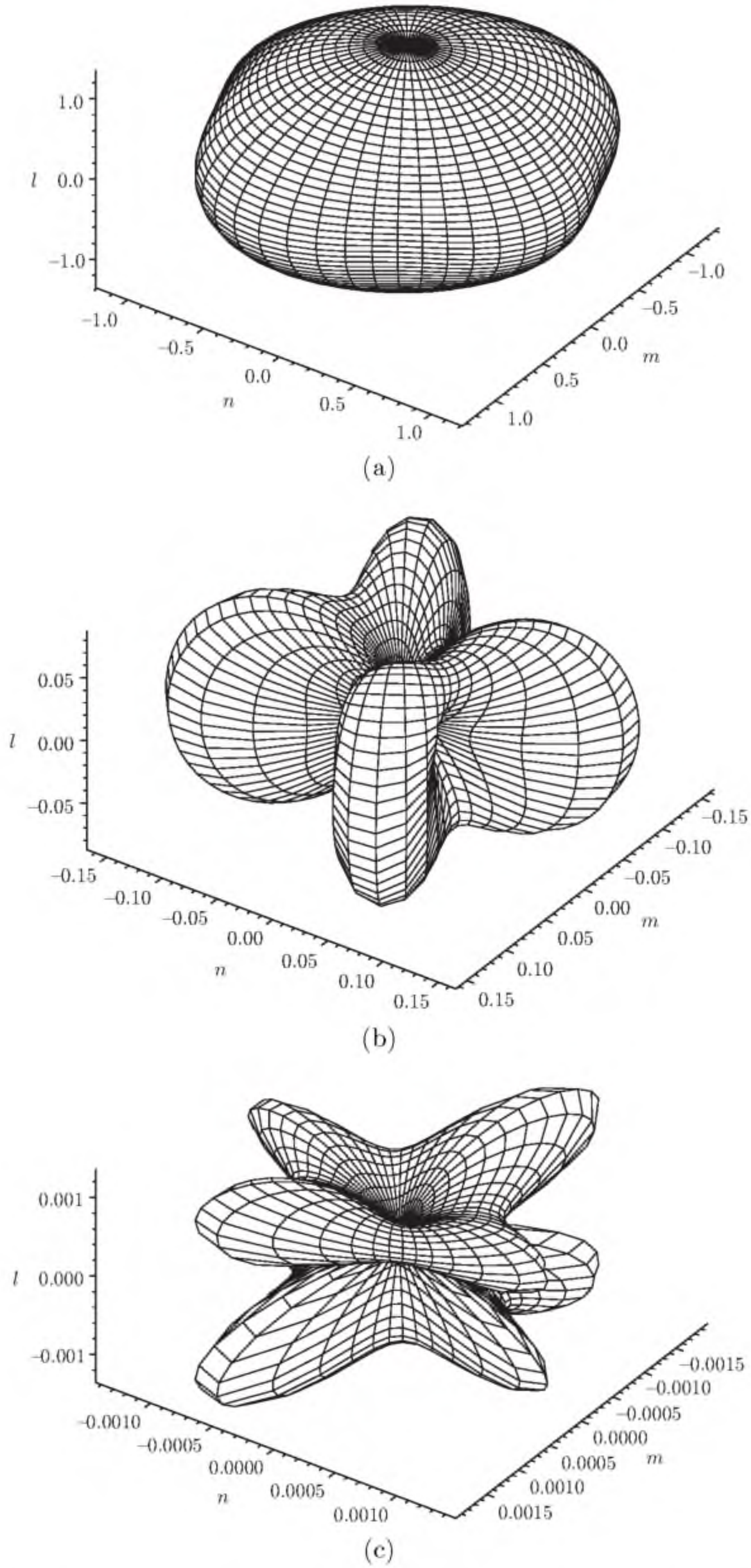

Fig. 2. Angle dependence of the velocity of the first (a), second (b), and third (c) sounds for the parameter values $\lambda_1 = 0.1$, $\lambda_2 = 0.2$, and $\lambda_3 = 0.05$.

where $q = I_2 - I_4^2/3$ and $t = 2I_4^3/27 - I_2 I_4/3 + I_0$. The real solutions of the reduced equation are

$$y_k = \sqrt{\frac{4}{3}\left(\frac{1}{3}I_4^2 - I_2\right)}\cos\left(\frac{\phi}{3} + (k-1)\frac{2\pi}{3}\right), \quad k = 1, 2, 3,$$

where

$$\cos\phi = -\frac{1}{2\rho}\left(\frac{2}{27}I_4^3 - \frac{1}{3}I_2 I_4 + I_0\right), \qquad \rho = \left[\frac{1}{3}\left(\frac{1}{3}I_4^2 - I_2\right)\right]^{3/2}.$$

For the original equation (4.11), we obtain the respective solutions

$$\Omega_k^2 = y_k - \frac{I_4}{3}, \quad k = 1, 2, 3.$$

The three branches of the acoustic spectra Ω_k^2, $k = 1, 2, 3$, are shown in Fig. 2.

In this paper, we have shown that using the Hamiltonian formalism permits making the functional hypothesis for biaxial liquid crystals more precise. Because of the closure requirement on the Poisson bracket algebra, we must introduce additional reduced-description parameters, i.e., conformational degrees of freedom. As a result, we predict that there exists a reactive component of the second sound in nematic liquid crystals with disklike molecules and demonstrate that the second and third sounds can propagate in biaxial nematics with rodlike molecules.

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