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## DYNAMICS OF BIAXIAL NEMATIC LIQUID CRYSTALS WITH CONFORMATIONAL DEGREES OF FREEDOM

A.P. IVASHIN, M.Yu. KOVALEVSKY, L.V. LOGVINOVA<sup>1</sup>,  
V.T. MATSKEVICH

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National Scientific Center “Kharkiv Institute of Physics and Technology”  
(1, Akademichna Str., Kharkiv 61108, Ukraine; e-mail: ivashin@kipt.kharkov.ua),

<sup>1</sup>Belgorod State University  
(85, Pobedy Str., Belgorod, Russia)

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On the basis of the Hamilton approach, the dynamics of biaxial nematic liquid crystals is considered, and the nonlinear equations of ideal hydrodynamics for such condensed media are deduced. The connection of the disk-like form of molecules and the structure of these equations is studied. Two branches of acoustic oscillations are found, and the character of an anisotropy of both sound velocities is clarified. In both cases, the computer simulation of a wave propagation front is performed.

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### Introduction

In the phenomenological approach, the equations of the dynamics of liquid crystals are deduced from the concepts of symmetry with regard for the conservation laws [1 — 3]. In this case, we are faced with the problem of accurate account of nonlinear terms in these equations. The Hamilton approach as an efficient method of construction of the dynamical equations describing the transfer phenomena in various condensed media seems to be more successive [4 — 7]. In the Hamilton approach, the basic role is played by the structure of Poisson brackets (PB) for the reduced description parameters which set a medium state in a macroscopically full manner.

In condensed media with a spontaneously broken symmetry, the choice of reduced description parameters depends on a number of factors. A part of hydrodynamic parameters is related to the symmetry properties of the Hamiltonian, which is manifested by the presence of the dynamical equations defined by differential conservation laws. Another factor influencing the composition of

hydrodynamic parameters is a form of molecules. In liquid crystals, the latter is connected with the structure of hydrodynamic equations. As shown in works [8 — 10], the structure of the PB of hydrodynamic parameters is different for disk-like and rod-like molecules. The physical manifestations of the influence of a form of molecules are different signs of the reactive coefficient in hydrodynamic equations [11], different possibilities to realize the ferroelectric state [12, 13], and spectral peculiarities of the polarization absorption of light [14]. In work [15], a certain peculiarity of the connection of a form of molecules and the hydrodynamics of biaxial nematics is clarified. It reveals itself, first, in the different structures of PB for the reduced description parameters and, secondly, in the necessity to increase the number of reduced description parameters on the hydrodynamic stage of evolution. From the mathematical viewpoint, the appearance of an additional quantity is conditioned by the requirement for the PB algebra to be closed for the entire collection of hydrodynamic variables. From the physical viewpoint, this fact is related to the presence of several characteristic lengths and times of relaxation in such a medium which are caused by the conformational flexibility of molecules.

As last, the collection of parameters is connected with the character of the spontaneous breaking of a symmetry of the system. The statement of elasticity theory as a part of continuum mechanics is based on the idea of spontaneously broken translational symmetry. In the collection of reduced description parameters, the dynamical quantity related to such a symmetry breaking is the strain tensor which is represented in terms of the

distortion tensor [16]. The latter quantity completely reflects the character of deformations of a continuum. However, its introduction as an additional quantity is, as a rule, excessive. The hydrodynamic theory of liquid crystals is also the mechanics of a continuum with spontaneously broken symmetry. In this case, the equilibrium state symmetry relative to rotations and shifts in the configuration space is broken. It was shown in works [10, 15] that the additional hydrodynamic parameters related to such a symmetry breaking can be also represented in terms of the distortion tensor for a number of uniaxial and biaxial liquid crystals.

In works [17 – 19], the hydrodynamics of biaxial liquid crystals was analyzed. This class of liquid crystals is characterized by the complete spontaneous breaking of the symmetry relative to rotations in the configuration space  $O(3)$ . However, these works do not contain explicitly the expressions for all the reactive densities of the flows of additive integrals of motion in terms of the energy functional and do not reveal the character of the influence of a form of molecules on the dynamical equations.

The present work defines more exactly the functional hypothesis on the basis of the developed Hamilton approach. The additional quantities related to a spontaneous breaking of the symmetry relative to rotations in the configurational space are introduced in terms of the distortion tensor. The densities and flows of additive integrals of motion are represented in terms of the energy density, the equations of ideal hydrodynamics are deduced, and the spectra of collective excitations of biaxial liquid crystals with regard for the conformational flexibility of molecules are investigated.

## 1. Differential Conservation Laws

The Hamilton approach for systems with the continual number of degrees of freedom was rather adequately studied in works [4, 6].

We introduce the distortion tensor as

$$b_{ki}(x) \equiv \delta_{ki} - \nabla_i u_k(x). \quad (1)$$

It is defined in terms of the shift vector  $u_k(x)$  which connects the Lagrange coordinate  $\xi_k$  with the Euler coordinate  $x_k$ ,

$$x_k = \xi_k + u_k(x).$$

The distortion tensor  $b_{ki}(x)$  [16] sets the orientational and translational states of equilibrium and defines the group of motions of a nonequilibrium state of the

continuum. We define the density  $\rho(x)$  of the substance in an arbitrary state in terms of the distortion tensor by the equality [6]

$$\rho(x) = \underline{\rho} \det |b_{ij}(x)|, \quad (2)$$

where  $\underline{\rho}$  is the substance density in a strainless state.

As known, the equation of motion for the density  $a(x)$  of an arbitrary physical quantity can be represented as [23]:

$$\dot{a}(x) = \{a(x), H\} \equiv \{A, \varepsilon(x)\} - \nabla_k a_k(x), \quad (3)$$

where  $A = \int d^3x a(x)$ ,  $H = \int d^3x \varepsilon(x)$ ,

$$a_k(x) = \int d^3x' x'_k \times \int_0^1 d\lambda \{a(x + \lambda x'), \varepsilon(x - (1 - \lambda)x')\}.$$

Below, we present the densities of flows of the relevant densities of additive integrals of motion. Let  $a(x) = \rho(x)$ . Then, taking into account that

$$M = \int d^3x \rho(x), \quad \{M, \varepsilon(x)\} = 0,$$

we get the differential law of conservation of the mass:

$$\dot{\rho}(x) = -\nabla_k j_k(x), \quad (4)$$

$$j_k(x) = \int d^3x' x'_k \times \int_0^1 d\lambda \{\rho(x + \lambda x'), \varepsilon(x - (1 - \lambda)x')\}.$$

Here,  $j_k(x)$  is the mass flow density. We set  $a(x) = \pi_k(x)$ , where  $\pi_k(x)$  is the momentum density. With regard for the translational invariance of the energy density

$$P_i = \int d^3x \pi_i(x), \quad \{P_i, \varepsilon(x)\} = \nabla_i \varepsilon(x),$$

we get the differential law of conservation of the momentum:

$$\dot{\pi}_i(x) = -\nabla_k t_{ik}(x), \quad (5)$$

$$t_{ik}(x) = -\varepsilon(x) \delta_{ik} + \int d^3x' x'_k \times$$

$$\times \int_0^1 d\lambda \{ \pi_i(x + \lambda x'), \varepsilon(x - (1 - \lambda)x') \},$$

where  $t_{ik}(x)$  is the momentum flow density. For  $a(x) = \varepsilon(x)$ , relation (3) yields the differential law of conservation of the energy:

$$\dot{\varepsilon}(x) = -\nabla_k q_k(x), \quad (6)$$

$$q_k(x) = \frac{1}{2} \int d^3x' x'_k \times$$

$$\times \int_0^1 d\lambda \{ \varepsilon(x + \lambda x'), \varepsilon(x - (1 - \lambda)x') \},$$

where  $q_k(x)$  is the energy flow density.

It is known that the PB for the densities of momentum, number of particles, entropy  $s(x)$ , and the distortion tensor are as follows [10]:

$$\{ \pi_i(x), s(x') \} = -s(x) \nabla_i \delta(x - x'),$$

$$\{ \pi_i(x), b_{kj}(x') \} = -b_{ki}(x') \nabla_j \delta(x - x'),$$

$$\{ \pi_i(x), \pi_j(x') \} = \pi_j(x) \nabla'_i \delta(x - x') - \pi_i(x') \nabla_j \delta(x - x'),$$

$$\{ \pi_i(x), \rho(x') \} = -\rho(x) \nabla'_i \delta(x - x'). \quad (7)$$

These PB serve as a basis for the construction of nonlinear equations of the hydrodynamic type for normal liquids, crystals, and liquid crystals. Further, we take into account that the Hamiltonian of the system has the Galilei-invariant form

$$H = \int d^3x \left( \frac{\pi_i^2(x)}{2\rho(x)} + \Phi(\rho, s, b_{ij}) \right). \quad (8)$$

In this case,  $m_{jk} = \pi_k$ .

## 2. Dynamics of Biaxial Nematic Liquid Crystals

Consider the condensed media with the spontaneously broken symmetry relative to rotations in the configurational space. This class of condensed media includes nematic liquid crystals. We note preliminarily that the state of an isotropic liquid is described with such macroscopic dynamical variables as the mass density  $\rho(x)$ , momentum density  $\pi(x)$ , and entropy density  $s(x)$ . The nematic phase of liquid crystals cannot be adequately described with these parameters, because this state is characterized by a spontaneous breaking

of the rotational symmetry which is conditioned by an anisotropy of molecules. In [21], the Hamilton approach was used for the description of the hydrodynamics of uniaxial nematics with one conformational degree of freedom. A representation of additional hydrodynamic parameters in terms of the distortion tensor for biaxial nematics with regard for one conformational degree of freedom is given in [22]. In the present work, by considering the dynamics of biaxial liquid crystals in the frame of the Hamilton approach, we restrict ourselves by the case of disk-like molecules. The unit and orthogonal axes of anisotropy which characterize a breaking of the rotational invariance,  $\vec{m}(x)$ ,  $\vec{n}(x)$ , are defined by the equalities

$$n_i(x) \equiv \frac{a(x)b_i(x) + b(x)a_i(x)}{|a(x)\vec{b}(x) + b(x)\vec{a}(x)|},$$

$$m_i(x) \equiv \frac{a(x)b_i(x) - b(x)a_i(x)}{|a(x)\vec{b}(x) - b(x)\vec{a}(x)|}. \quad (9)$$

The vectors  $\vec{a}(x)$  and  $\vec{b}(x)$  can be written in terms of the distortion tensor as follows:

$$a_j(x) \equiv e_{1k} b_{kj}(x), \quad b_j(x) \equiv e_{2k} b_{kj}(x). \quad (10)$$

Here,  $e_{1k}, e_{2k}$  are the unit orthogonal constant vectors setting the directions of the anisotropy axes of a strainless state, and  $a(x) = |\vec{a}(x)|$ ,  $b(x) = |\vec{b}(x)|$  are the lengths of these axes in a deformed state. The unit vectors  $\vec{m}(x), \vec{n}(x)$  set anisotropic properties of the medium related to the anisotropy of the properties of molecules. According to formulas (9), (10), (7), we get the PB for  $\pi_k, n_k, m_k$ :

$$\{ \pi_i(x), n_j(x') \} =$$

$$= \delta(x - x') \nabla_i n_j(x) + f_{i\lambda j}(x') \nabla'_\lambda \delta(x - x'),$$

$$\{ \pi_i(x), m_j(x') \} =$$

$$= \delta(x - x') \nabla_i m_j(x) + g_{i\lambda j}(x') \nabla'_\lambda \delta(x - x'). \quad (11)$$

The functions  $f_{i\lambda j}(x), g_{i\lambda j}(x)$  in (11) are defined by the equalities

$$f_{i\lambda j}(x) \equiv n_i \delta_{j\lambda}^\perp(\vec{n}(x)) -$$

$$- p(x) m_j(x) [n_i(x) m_\lambda(x) + n_\lambda(x) m_i(x) t],$$

$$g_{i\lambda j}(x) \equiv m_i \delta_{j\lambda}^\perp(\vec{m}(x)) -$$

$$- (1 - p(x)) n_j(x) [n_i(x) m_\lambda(x) + n_\lambda(x) m_i(x)],$$

$$\delta_{kj}^\perp(f(x)) \equiv \delta_{kj} - f_k(x)f_j(x).$$

We see that the right-hand side of PB (11) contains the quantity

$$p(x) \equiv \frac{1}{2} \left( 1 - \frac{\vec{a}(x)\vec{b}(x)}{a(x)b(x)} \right). \quad (12)$$

Thus, in order to close the algebra of PB for the liquid crystals under study, it is necessary to expand the collection of reduced description parameters by including the quantity  $p(x)$  in it. In the general case for biaxial liquid crystals, it is possible to introduce three conformational degrees of freedom representable in terms of the distortion tensor. One of them is defined by equality (12), and the two others are defined by the relations

$$\begin{aligned} \bar{a}(x) &\equiv 2|\vec{a}(x)|(1-p(x))^{1/2}, \\ \bar{b}(x) &\equiv 2|\vec{b}(x)|p(x)^{1/2}. \end{aligned} \quad (13)$$

Directions of the vectors  $\vec{a}$  и  $\vec{b}$  and their moduli  $|\vec{a}(x)|$ ,  $|\vec{b}(x)|$  take into account, respectively, the orientation of molecules and their size. The scalar parameter  $p(x)$  is defined by the angle between the deformed axes of a liquid crystal. On the macroscopic level of description, the conformational parameters  $\bar{a}$ ,  $\bar{b}$ ,  $p$  reflect the influence of the form and size of molecules of a liquid crystal on the structure of the equations of hydrodynamics.

From definitions (12), (13) with regard for (10), (7), we get the PB for the conformational degrees of freedom and the momentum density,

$$\begin{aligned} \{\pi_i(x), p(x')\} &= \\ &= \delta(x-x')\nabla_i p(x) + h_{il}(x')\nabla'_l \delta(x-x'), \\ \{\pi_i(x), \bar{a}(x')\} &= \\ &= \delta(x-x')\nabla_i \bar{a}(x) + f_{ij}(x')\nabla_j \delta(x-x'), \\ \{\pi_i(x), \bar{b}(x')\} &= \\ &= \delta(x-x')\nabla_i \bar{b}(x) + g_{ij}(x')\nabla_j \delta(x-x'), \end{aligned} \quad (14)$$

where we use the following notations:

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

$$h_{ik} = 2p(1-p)(m_i m_k - n_i n_k). \quad (15)$$

The orientational and conformational degrees of freedom  $\vec{m}(x)$ ,  $\vec{n}(x)$ ,  $\bar{a}(x)$ ,  $\bar{b}(x)$ ,  $p(x)$  are local functions of the distortion tensor and are considered as independent variables. The PB (7), (11), (14) form a closed algebra of hydrodynamic variables for a biaxial nematic with disk-like molecules.

With regard for the PB (7), (11), (14), the equation of motion in the Hamilton form (1) yields the equations of motion for a biaxial nematic with disk-like molecules,

$$\begin{aligned} \dot{s}(x) &= -\nabla_i(s(x)v_i(x)), \quad \dot{\rho}(x) = -\nabla_i \pi_i(x), \\ \dot{\pi}_i(x) &= -\nabla_k t_{ik}(x), \\ \dot{n}_j(x) &= -v_s(x)\nabla_s n_j(x) - f_{i\lambda j}(x)\nabla_\lambda v_i(x), \\ \dot{m}_j(x) &= -v_s(x)\nabla_s m_j(x) - g_{i\lambda j}(x)\nabla_\lambda v_i(x), \\ \dot{p}(x) &= -v_s(x)\nabla_s p(x) - h_{ij}(x)\nabla_i v_j(x), \\ \dot{\bar{a}}(x) &= -v_i(x)\nabla_i \bar{a}(x) - f_{ij}(x)\nabla_i v_j(x), \\ \dot{\bar{b}}(x) &= -v_i(x)\nabla_i \bar{b}(x) - g_{ij}(x)\nabla_i v_j(x), \end{aligned} \quad (16)$$

where  $v_i(x) = \pi_i(x)/\rho(x) \equiv \partial\varepsilon(x)/\partial\pi_i(x)$  is the motion velocity of a unit mass of the medium. The momentum flow density  $t_{ik}(x)$  can be found with the use of the collection of PB (7), (11), (14) and formula (5) and can be represented in terms of the energy density as

$$\begin{aligned} t_{ik} &= t_{ik}^o + t'_{ik}, \\ t_{ik}^o &= \frac{\pi_i \pi_k}{\rho} + \left( \sigma \frac{\partial\Phi}{\partial\sigma} + \rho \frac{\partial\Phi}{\partial\rho} - \Phi \right) \delta_{ik}, \\ t'_{ik} &= \frac{\partial\varepsilon}{\partial\nabla_k n_j} \nabla_i n_j + \frac{\partial\varepsilon}{\partial\nabla_k m_j} \nabla_i m_j + \\ &+ f_{ikl} \left( \frac{\partial\varepsilon}{\partial n_l} - \nabla_j \frac{\partial\varepsilon}{\partial\nabla_j n_l} \right) + g_{ikl} \left( \frac{\partial\varepsilon}{\partial m_l} - \nabla_j \frac{\partial\varepsilon}{\partial\nabla_j m_l} \right) + \\ &+ \frac{\partial\varepsilon}{\partial p} h_{ik} + \frac{\partial\varepsilon}{\partial \bar{a}} f_{ik} + \frac{\partial\varepsilon}{\partial \bar{b}} g_{ik}. \end{aligned} \quad (17)$$

The second principle of thermodynamics with regard for (15) reads

$$\begin{aligned} d\varepsilon &= \mu dp + \rho T d\sigma + v_i d\pi_i + \left( \frac{\partial\varepsilon}{\partial n_i} - \nabla_j \frac{\partial\varepsilon}{\partial\nabla_j n_i} \right) \times \\ &\times \delta_{ik}^\perp(\vec{n}) dn_k + \frac{\partial\varepsilon}{\partial p} dp + \frac{\partial\varepsilon}{\partial \bar{a}} d\bar{a} + \frac{\partial\varepsilon}{\partial \bar{b}} d\bar{b} + \end{aligned}$$

$$\begin{aligned}
& + \left( \frac{\partial \varepsilon}{\partial m_i} - \nabla_j \frac{\partial \varepsilon}{\partial \nabla_j m_i} \right) \delta_{ik}^\perp(\vec{m}) dm_k + \\
& + \nabla_j \left( \frac{\partial \varepsilon}{\partial \nabla_j n_i} \delta_{ik}^\perp(\vec{n}) dn_k + \frac{\partial \varepsilon}{\partial \nabla_j m_i} \delta_{ik}^\perp(\vec{m}) dm_k \right), \quad (18)
\end{aligned}$$

where  $T$  is the temperature and  $\mu$  is the chemical potential. The energy flow density is defined from Eqs. (11), (13), (7) with regard for (6) and takes the form

$$\begin{aligned}
\dot{\varepsilon} &= -\nabla_k q_k, \quad q_k = q_k^0 + q_k' + q_k'', \\
q_k^0 &= \frac{\partial \varepsilon}{\partial \pi_k} \left( \rho \frac{\partial \varepsilon}{\partial \rho} + s \frac{\partial \varepsilon}{\partial s} + \pi_i \frac{\partial \varepsilon}{\partial \pi_k} \right), \quad q_k' = \frac{\partial \varepsilon}{\partial \pi_k} t'_{ik}, \\
q_k'' &= \left( \frac{\partial \varepsilon}{\partial \nabla_k n_i} f_{jil} + \frac{\partial \varepsilon}{\partial \nabla_k m_i} g_{jil} \right) \nabla_l \frac{\partial \varepsilon}{\partial \pi_j}. \quad (19)
\end{aligned}$$

We note that formulas (16) are the complete collection of equations of the ideal hydrodynamics of a biaxial nematic which consists of disk-like molecules with three conformational degrees of freedom. Further, we use these equations in the derivation of the spectra of collective excitations of biaxial nematics which consist of disk-like molecules with one or three conformational degrees of freedom, respectively.

### 3. Spectra of Collective Excitations of Biaxial Nematics

By using the deduced equations for a biaxial nematic (16), we study the spectra of collective excitations. We assume that the medium is homogeneous and strainless ( $p = 1/2$ ) in the equilibrium state and immovable as a whole ( $v_k = 0$ ). This means that

$$\begin{aligned}
\frac{\partial \varepsilon}{\partial n_k} &= \frac{\partial \varepsilon}{\partial \nabla_l n_k} = \frac{\partial^2 \varepsilon}{\partial n_k \partial \nabla_l n_j} = 0, \\
\frac{\partial \varepsilon}{\partial m_k} &= \frac{\partial \varepsilon}{\partial \nabla_l m_k} = \frac{\partial^2 \varepsilon}{\partial m_k \partial \nabla_l m_j} = 0, \\
\frac{\partial \varepsilon}{\partial v_k} &= \frac{\partial^2 \varepsilon}{\partial v_j \partial n_k} = \frac{\partial^2 \varepsilon}{\partial v_k \partial \nabla_l n_j} = 0. \quad (20)
\end{aligned}$$

As a result of the linearization of the system of equations (16), we get the equations describing small deviations of the parameters of a biaxial nematic from the equilibrium position,

$$\begin{aligned}
\delta \dot{n} &= -n \nabla_j v_j, \quad \delta \dot{s} = 0, \quad \delta \dot{p} = \frac{1}{2} (n_i n_i - m_i m_i) \nabla_i v_i, \\
mn \delta \dot{v}_i &= \frac{\partial P}{\partial n} \nabla_i n + \frac{1}{2} (n_i n_i - m_i m_i) \times \\
&\times \left[ \frac{\partial^2 \varepsilon}{\partial p^2} \nabla_i \delta p + \frac{\partial^2 \varepsilon}{\partial p \partial n} \nabla_i \delta n \right],
\end{aligned}$$

$$\begin{aligned}
\delta \dot{n}_j &= \left[ -n_i \delta_{\lambda j}^\perp(\vec{n}) + \frac{1}{2} (n_\lambda m_i + n_i m_\lambda) \right] \nabla_\lambda \delta v_i, \\
\delta \dot{m}_j &= \left[ -m_i \delta_{\lambda j}^\perp(\vec{m}) + \frac{1}{2} (n_\lambda m_i + n_i m_\lambda) \right] \nabla_\lambda \delta v_i, \quad (21)
\end{aligned}$$

where  $m$  — molecule mass and  $n$  — density. In the derivation of the system of equations (21), we took into account that, according to (12), a minimum is present at the point  $p = 1/2$  in the strainless state, i.e.,  $\left( \frac{\partial \varepsilon}{\partial p} \right)_{p=1/2} = 0$ . In addition, we consider the term  $\frac{\partial^2 \varepsilon}{\partial p \partial n}$  to be small as compared to  $\frac{\partial^2 \varepsilon}{\partial p^2}$ . From the system of equations (21), we obtained the values of linear deviations of the density  $\delta n$  and the parameter  $\delta p$  from their equilibrium values and substituted them into the linearized equation for deviations of the velocity  $\delta v_i$ . As the result, we got the dispersion equation for the determination of the spectra of collective excitations:

$$\det \left( \omega^2 \delta_{ij} - k_i k_j \frac{\partial P}{\partial \rho} - D_i^\alpha(\vec{k}) D_j^\alpha(\vec{k}) \right) = 0,$$

where

$$D_i^\alpha(\vec{k}) \equiv \left( \sqrt{A} f_i, \sqrt{B} g_i, \sqrt{C} h_i \right),$$

$$f_i(k) \equiv f_{il} k_l, \quad g_i(k) \equiv g_{il} k_l, \quad h_i(k) \equiv h_{il} k_l,$$

$$A \equiv \frac{1}{\rho} \frac{\partial^2 \varepsilon}{\partial a^2}, \quad B \equiv \frac{1}{\rho} \frac{\partial^2 \varepsilon}{\partial b^2}, \quad C \equiv \frac{1}{\rho} \frac{\partial^2 \varepsilon}{\partial p^2}.$$

The quantity  $D_i^\alpha(\vec{k})$  defines the corrections to the acoustic spectrum of a biaxial nematic which was derived without taking a form of molecules into account.

By developing the determinant, we arrive at the equation

$$\omega^2 (\omega^4 + \omega^2 L_4(\theta, \varphi) + L_2(\theta, \varphi)) = 0. \quad (22)$$

Here, we used the notations

$$L_4(\theta, \varphi) = -k^2 c^2 - k^2 c^2 \sin^2 \theta \Phi(\theta, \varphi),$$

$$L_2(\theta, \varphi) = \Phi(\theta, \varphi) \sin^2 \theta + \sin^4 \theta \left[ -\Phi(\theta, \varphi) + \right.$$

$$\left. + (\lambda_a + \lambda_b) \frac{1 + \sin 4\varphi}{4} + \right.$$

$$\left. + \lambda_a \lambda_b \frac{1 + \sin 4\varphi}{4} + \lambda_a \lambda_c \left( \frac{1 - \sin 2\varphi}{2} \right)^2 + \right.$$

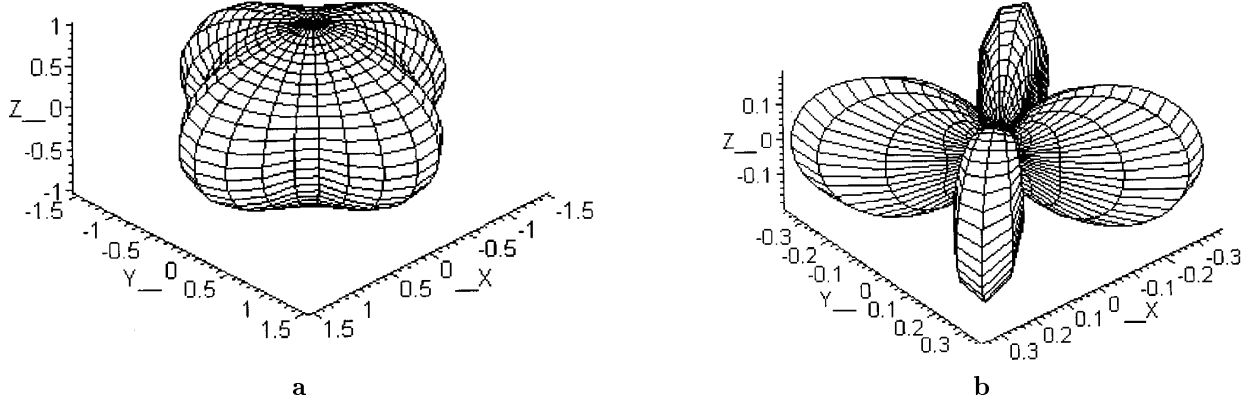


Fig.1. Velocities  $\tilde{c}_+$  (a) and  $\tilde{c}_-$  (b) vs angles at the parameter  $\lambda_c = 0.5$

$$+\lambda_b \lambda_c \left[ \frac{1 + \sin 2\varphi}{2} \right]^2 + \lambda_c \sin^2 2\varphi \Big],$$

$\Phi(\theta, \varphi) \equiv$

$$\equiv \left[ \frac{3}{4}(\lambda_a + \lambda_b) - (\lambda_a - \lambda_b) \frac{\sin 2\varphi - \cos 2\varphi}{2} + \lambda_c \right],$$

where

$$\lambda_a \equiv A/c^2, \quad \lambda_b \equiv B/c^2, \quad \lambda_c \equiv C/c^2, \quad c^2 \equiv \frac{\partial P}{\partial \rho}.$$

In the derivation of the dispersion equation (22), we used the relation

$$\det D_l^\alpha D_l^\alpha = \frac{1}{6} \varepsilon_{pqt} \varepsilon_{ikl} D_i^\alpha D_k^\beta D_l^\gamma D_p^\alpha D_q^\beta D_l^\gamma = 0$$

by virtue of the property  $D_i^\alpha \approx () n_i + () m_i$ .

Thus, two branches of acoustic oscillations corresponding to the first or second sound can propagate in a biaxial nematic:

$$\omega_\pm^2(\vec{k}) = \frac{1}{2} \left( -L_4(\vec{k}) \pm \sqrt{L_4^2(\vec{k}) - 4L_2(\vec{k})} \right),$$

$$\omega_\pm^2(\vec{k}) \equiv k^2 c_\pm^2(\vec{e}), \quad \vec{e} \equiv \vec{k}/k. \quad (23)$$

Here, the solution with sign (+) defines the sound which is analogous to that present in a normal liquid, whereas the solution with sign (-) defines the second sound, namely a new branch of excitations caused by the biaxiality of a liquid crystal and by the existence of the conformational degree of freedom for such liquid-crystalline states. It is clear that both solutions are characterized by an anisotropy of sound velocities. In

the spherical coordinate system,  $\vec{e}\vec{m} = \sin \theta \cos \varphi$ ,  $\vec{e}\vec{n} = \sin \theta \sin \varphi$ ,  $\vec{e}\vec{l} = \cos \theta$ , where  $\theta, \varphi$  are, respectively, the polar and azimuth angles setting a direction of the wave vector  $\vec{e}$ . In terms of these variables, the dimensionless velocities  $\tilde{c}_\pm(\theta, \varphi) \equiv c_\pm(\theta, \varphi)/c$  (23) ( $c$  is the sound velocity in the isotropic phase of the condensed medium under study) in a biaxial nematic with one conformational degree of freedom are

$$\tilde{c}_\pm(\theta, \varphi) = \frac{1}{\sqrt{2}} \left\{ 1 + \lambda_c \sin^2 \theta \pm \left[ (1 - \lambda_c \sin^2 \theta)^2 + 4\lambda_c \sin^4 \theta \cos^2 2\varphi \right]^{1/2} \right\}^{1/2} \quad (24)$$

Setting the parameter  $\lambda_c$  to be small, we decompose expression (24) in it. In the principal approximation in  $\lambda_c$ , we get

$$\tilde{c}_+(\theta, \varphi) \approx (1 + 0.5\lambda_c \sin^4 \theta \cos^2 2\varphi),$$

$$\tilde{c}_-(\theta, \varphi) \approx \sqrt{\lambda_c} |\sin \theta| \sqrt{1 - \sin^2 \theta \cos^2 2\varphi}. \quad (25)$$

In the directions  $\theta = 0, \pi$ , the second sound is absent, and the velocity of the first one coincides with that without regard for a form of molecules. At  $\theta = \pi/2$  and  $\varphi = 0, \pi/2, \pi, 3\pi/2$ , the dimensionless velocity of the first sound reaches the maximum value equal to  $1 + \lambda_c/2$ . The dimensionless velocity of the second sound is maximum in the directions  $\varphi = \pi/4, 3\pi/4, 5\pi/4, 7\pi/4$  and is equal to  $\sqrt{\lambda_c}$ .

Fig. 1 shows the character of an anisotropy of the velocities  $\tilde{c}_\pm(\theta, \varphi)$  (24). Three vectors  $\vec{m}, \vec{n}, \vec{l}$  form a rectangular Cartesian coordinate system (in the figures, for clearness, we drew the Cartesian coordinate system, where the vector  $\vec{l}$  is directed along the  $Z$  axis).

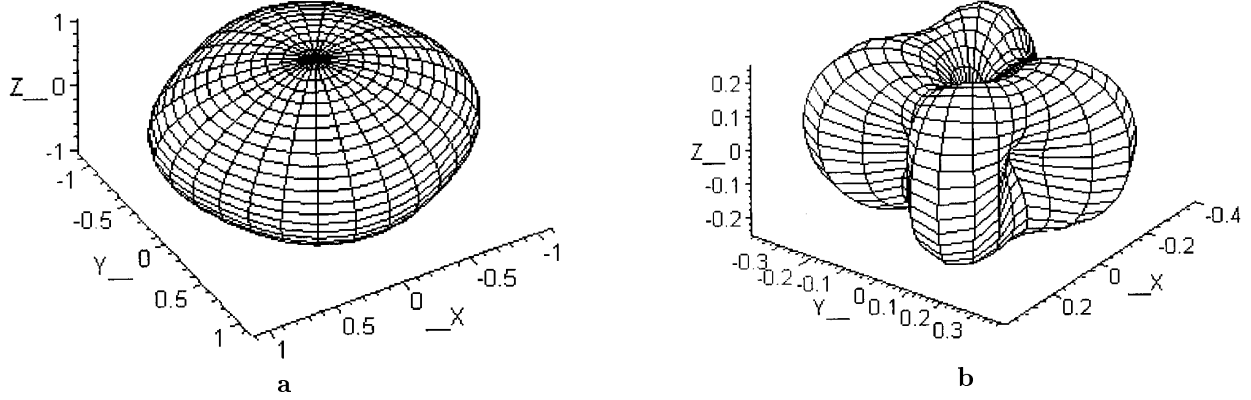


Fig.2. Velocities  $\tilde{c}_+$  (a) and  $\tilde{c}_-$  (b) vs angles at the parameters  $\lambda_a = 0.1$ ;  $\lambda_b = 0.2$ ;  $\lambda_c = 0.05$

With regard for three conformational degrees of freedom, relation (23) yields

$$\begin{aligned} \tilde{c}_{\pm}^2(\theta, \varphi) = & \frac{1}{2} \{1 + \Phi \sin^2 \theta\} \pm \frac{1}{2} \left\{ \{1 - \Phi \sin^2 \theta\}^2 + \right. \\ & + 4 \sin^4 \theta \left[ \Phi(\theta, \varphi) - (\lambda_a + \lambda_b) \frac{1 + \sin 4\varphi}{4} - \right. \\ & - \lambda_a \lambda_b \frac{1 + \sin 4\varphi}{4} - \lambda_a \lambda_c \left( \frac{1 - \sin 2\varphi}{2} \right)^2 - \\ & \left. \left. - \lambda_b \lambda_c \left( \frac{1 + \sin 2\varphi}{2} \right)^2 - \lambda_c \sin^2 2\varphi \right] \right\}^{1/2}. \end{aligned} \quad (26)$$

The dependence of the velocities  $\tilde{c}_+$  and  $\tilde{c}_-$  on angles is presented in Fig. 2 for the parameters  $\lambda_a = 0.1$ ;  $\lambda_b = 0.2$ ;  $\lambda_c = 0.05$ . As seen, the first sound velocity is that without regard for a form of molecules in the directions  $\theta = 0, \pi$ , and the second sound velocity tends to zero. The azimuth angular dependences of the velocities of first and second sounds for  $\theta = \pi/2$  are analogous to the previous case with one conformational degree of freedom.

The additional modes, which are related to the broken symmetry relative to rotations in the configurational space and manifest the dissipative character without a reactive component, were discovered in works [17–20]. By comparing our results with those of these works, we note that the account of the conformational degrees of freedom  $p, \bar{a}, \bar{b}$  in the hydrodynamic equations of a biaxial nematic leads to the appearance of a reactive component in the

spectrum of second sound already in the adiabatic approximation.

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ДИНАМІКА ДВОХОСНИХ НЕМАТИЧНИХ РІДКИХ КРИСТАЛІВ З КОНФОРМАЦІЙНИМИ СТУПЕНЯМИ ВІЛЬНОСТІ

*А.П.Івашин, М.Ю.Ковалевський, Л.В.Логвинова, В.Т.Мацкевич*

Резюме

На основі гамільтонова підходу розглянуто динаміку рідинно-кристалічної двохосної нематичної фази і виведено нелінійні рівняння ідеальної гідродинаміки. Вивчено зв'язок між дископодібною формою молекул та структурою гідродинамічних рівнянь. Знайдено дві гілки акустичних коливань для двохосних нематиків та визначено характер анізотропії обох швидкостей звуку.