Dynamics of nematics with conformational degrees of freedom

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Abstract

On the basis of Hamilton approach the dynamics of the biaxial nematics is considered. All hydrodynamic parameters, connected with broken symmetry, are introduced in terms of the distortion tensor. The equations of ideal hydrodynamics are obtained and the three spectra of collective excitations of biaxial nematics are considered, taking into account the rod-shape of molecules.

1. Introduction

Hamilton approach provides an effective method for construction of the non-linear dynamic equations describing the transport phenomena in various condensed media. The structure of Poisson brackets (PB) for reduced description parameters is playing the basic role in Hamilton approach. Selection of the reduced description parameters in the case of liquid crystals (LC) depends on a number of factors. Some hydrodynamic parameters are associated with the Hamiltonian symmetry properties, manifested as the presence of dynamic equations conditioned by the differential conservation laws. The molecular shape is another factor influencing the set of hydrodynamic parameters. There is a correlation between the molecular shape and the structure of hydrodynamic equations. The Poisson bracket structure of hydrodynamic parameters has been shown to be of different form for disc- and rod-shaped molecules [1–3]. In Refs. [4–8], a specific feature of the mentioned correlation between the molecular shape and hydrodynamics has been clarified.

The parameter set is associated with the character of spontaneous symmetry breaking in the system. The elasticity theory is formulated as part of the continuous medium mechanics, based on the concept of spontaneously broken translation symmetry. It is just the deformation tensor that represents the dynamic quantity in the set of reduced description parameters associated with such symmetry breaking. The LC hydrodynamic theory can also be viewed as continuous medium mechanics with spontaneously broken symmetry. In this case, there is the symmetry disturbance with respect to rotations in the configuration space. It has been shown [3,7] that additional hydrodynamic parameters associated with this symmetry disturbance can also be presented in terms of the distortion tensor for many uniaxial LC.

2. Poisson brackets in dynamical theory of liquid crystals

The dynamical equations for reduced description parameters $\varphi_\alpha(x)$ in Hamilton approach have the form

$$\varphi_\alpha(x) = \{\varphi_\alpha(x), H\}$$

here $H(\varphi)=\int d^3x\varepsilon(x, \varphi(x'))$ is the Hamiltonian of the system. The conservation laws in differential form are given by

$$\dot{\zeta}_a(x) = -\nabla_k \zeta_{ak}(x), \tag{1}$$

where $\zeta_a(x)\equiv\rho(x),\pi_i(x),\varepsilon(x)$ and $\zeta_{ak}(x)\equiv j_k(x),t_{ik}(x),q_k(x)$ are the density and flux density of additive integrals of motion: the mass, the momentum and the energy correspondingly. That can be presented in the terms of Poisson brackets for appropriate densities [9]:

$$\begin{aligned}
&\zeta_{ak}(x) = -\delta_{ak}\varepsilon(x) + \int d^3x' x'_k \int_0^1 d\lambda\{\zeta_a(y), \varepsilon(y', \zeta)\}, \quad a\neq 0,\\
&\zeta_{0k}(x) = \frac{1}{2}\int d^3x' x'_k \int_0^1 d\lambda\{\varepsilon(y,\zeta), \varepsilon(y',\zeta)\},\\
&(y\equiv x+\lambda x', y'\equiv x-(1-\lambda)x')
\end{aligned} \tag{2}$$

Let us write out PB for the momentum density $\pi_k(x)$, for the mass density $\rho(x)$, for the entropy density $\sigma(x)$ and distortion tensor $b_{ki}(x)$ in accordance to [3]

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

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

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

$$\{\pi_i(x), \rho(x')\} = \rho(x)\nabla'_j\delta(x-x'). \tag{3}$$

These PB are the bases of the construction of nonlinear equations of hydrodynamic type for the normal liquid, crystals and liquid crystals. The influence of the shape of molecule on dynamic properties is developed by means of different dependence of the energy on distortion tensor.

3. Dynamics of biaxial nematic crystals with rod-shaped molecules

In the case of biaxial rod-shaped molecules, lets introduce the unit and orthogonal anisotropy axes $\vec{m}(x)$, $\vec{n}(x)$ by formulae

$$n_i(x) = \frac{A(x)B_i(x) + B(x)A_i(x)}{|A(x)\vec{B}(x) + B(x)\vec{A}(x)|},$$
$$m_i(x) = \frac{A(x)B_i(x) - B(x)A_i(x)}{|A(x)\vec{B}(x) - B(x)\vec{A}(x)|}. \tag{4}$$

Here, the quantities $A_j(x)$ and $B_j(x)$ are defined in term of distortion tensor

$$A_j(x) \equiv e_{1k}b^{-1}_{kj}(x), \quad B_j(x) \equiv e_{2k}b^{-1}_{kj}(x), \tag{5}$$

e_{1k}, e_{2k} are the orthogonal vectors defining the anisotropy axes in the strain-free state.

Taking into account the definitions of Eqs. (4) and (5) and the PB set (Eq. (3)), we obtain the Poisson brackets

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

$$\{\pi_i(x), m_j(x')\} = \delta(x-x')\nabla_i m_j(x) + G_{i\lambda j}(x')\nabla'_\lambda\delta(x-x'), \tag{6}$$

where the following notations are used

$$F_{i\lambda j}(x) \equiv -n_\lambda(x)\delta^\perp_{ij}\left(\vec{n}(x)\right) + p(x)m_j(x)(n_i(x)m_\lambda(x) + n_\lambda(x)m_i(x)),$$

$$G_{i\lambda j}(x) \equiv -m_\lambda(x)\delta^\perp_{ij}\left(\vec{m}(x)\right) + (1-p(x))n_j(x)(n_i(x)m_\lambda(x) + n_\lambda(x)m_i(x)).$$

Let's introduce the conformational parameters $p(x)$, $\bar{A}(x)$, $\bar{B}(x)$

$$p(x) \equiv \frac{1}{2}\left(1 - \frac{\vec{A}(x)\vec{B}(x)}{A(x)B(x)}\right),$$

$$\overline{A}(x) \equiv 2A(x)(1-p(x))^{1/2}, \qquad \overline{B}(x) \equiv 2B(x)p^{1/2}(x).$$

The quantity $p(x)$ is defined by the angle between long and short axes of molecules of LC. The values $\bar{A}(x)$ and $\bar{B}(x)$ are

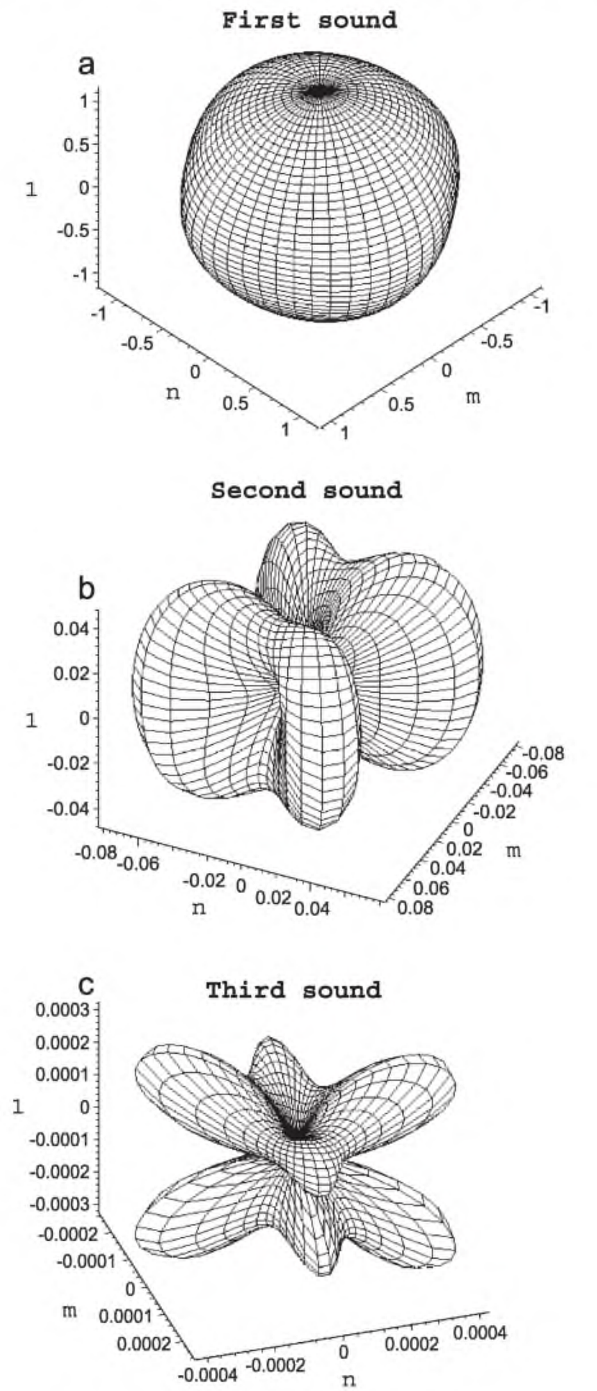

Fig. 1. The angular dependencies for dimensionless sound velocities $\tilde{c}_1(\theta,\varphi)$ (1a), $\tilde{c}_2(\theta,\varphi)$ (1b) and $\tilde{c}_3(\theta,\varphi)$ (1c) at λ_1=0.1, λ_2=0.02, λ_3=0.05.

connected with the size of the long and short axes of molecule in nondeformed equilibrium states. The Poisson brackets for these quantities are as follows

$$\{\pi_i(x),p(x')\} = \delta(x-x')\nabla_i p(x) + 2H_{ij}(x')\nabla'_j\delta(x-x'),$$

$$\{\pi_i(x),\bar{A}(x')\} = \delta(x-x')\nabla_i \bar{A}(x) + F_{ij}(x')\nabla'_j\delta(x-x'),$$

$$\{\pi_i(x),\bar{B}(x')\} = \delta(x-x')\nabla_i \bar{B}(x) + G_{ij}(x')\nabla'_j\delta(x-x'), \qquad (7)$$

where the following notations are used

$$F_{ik} = \bar{A}\left(\delta^{\perp}_{ik}\left(\vec{n}\right) - \sqrt{p(1-p)}(n_i m_k + n_k m_i)\right),$$
$$G_{ik} = \bar{B}\left(\delta^{\perp}_{ik}\left(\vec{m}\right) + \sqrt{p(1-p)}(n_i m_k + n_k m_i)\right),$$
$$H_{ik} = -2p(1-p)(m_i m_k - n_i n_k).$$

From Eqs. (1) and (2), in accordance to Eqs. (3), (6), and (7), we shall get the set of equations for the ideal hydrodynamics of biaxial nematic with the rod-shaped molecules

$$\frac{\partial\sigma(x)}{\partial t} = -\nabla_i(\sigma(x)v_i(x)),\ \frac{\partial\rho(x)}{\partial t} = -\nabla_i\pi_i(x),$$
$$\frac{\partial\pi_i(x)}{\partial t} = -\nabla_k t_{ik}(x),$$

$$t_{ik} = \delta_{ik}P + \frac{\partial\varepsilon}{\partial\pi_k}\pi_i + \frac{\delta H}{\delta n_l}F_{ikl} + \frac{\delta H}{\delta m_l}G_{ikl} + \frac{\partial\varepsilon}{\partial p}H_{ik}$$
$$+\frac{\partial\varepsilon}{\partial\bar{A}}F_{ik} + \frac{\partial\varepsilon}{\partial\bar{B}}G_{ik} + +\frac{\partial\varepsilon}{\partial\nabla_k n_j}\nabla_i n_j + \frac{\partial\varepsilon}{\partial\nabla_k m_j}\nabla_i m_j$$

$$P=\left(\frac{\partial\varepsilon}{\partial\rho}\rho + \frac{\partial\varepsilon}{\partial\pi_l}\pi_l + \frac{\partial\varepsilon}{\partial\sigma}\sigma - \varepsilon\right),\quad v_k = \frac{\partial\varepsilon}{\partial\pi_k},$$

$$\frac{\partial n_j(x)}{\partial t} = -v_s(x)\nabla_s n_j(x) - F_{i\lambda j}(x)\nabla_\lambda v_i(x),$$
$$\frac{\partial m_j(x)}{\partial t} = -v_s(x)\nabla_s m_j(x) - G_{i\lambda j}(x)\nabla_\lambda v_i(x),$$
$$\frac{\partial\bar{A}(x)}{\partial t} = -v_i(x)\nabla_i\bar{A}(x) - F_{ij}(x)\nabla_j v_i(x),$$
$$\frac{\partial\bar{B}(x)}{\partial t} = -v_i(x)\nabla_i\bar{B}(x) - G_{ij}(x)\nabla_j v_i(x),$$
$$\frac{\partial p(x)}{\partial t} = -v_s(x)\nabla_s p(x) - H_{kl}(x)\nabla_k v_l(x).$$

Linearization of these equations reduce to bicubic dispersion equation

$$\omega^6 + \omega^4 I_4(\theta,\varphi) + \omega^2 I_2(\theta,\varphi) + I_0(\theta,\varphi) = 0, \qquad (8)$$

where

$$I_4(\theta,\varphi) = -k^2c^2(1+\sin^2\theta)\left\{(\lambda_1+\lambda_2)\left(ctg^2\theta + \frac{3}{4}\right) + (\lambda_1-\lambda_2)\frac{\sin2\varphi-\cos2\varphi}{2} + \lambda_3\right\},$$

$$I_2(\theta,\varphi) = k^4c^4\left\{\sin^2\theta\left\{(\lambda_1+\lambda_2)\left(ctg^2\theta+\frac{3}{4}\right) + (\lambda_1-\lambda_2)\times\frac{\sin2\varphi-\cos2\varphi}{2} + \lambda_3\right\} + \sin^4\theta x \times\left\{\lambda_1\lambda_2\left[2ctg^2\theta + \frac{1+\sin4\varphi}{4}\right] + \lambda_1\lambda_3\left[ctg^2\theta + \left(\frac{1+\sin2\varphi}{2}\right)^2\right] + \lambda_2\lambda_3\left[ctg^2\theta + \left(\frac{1-\sin2\varphi}{2}\right)^2\right] - (\lambda_1+\lambda_2)\times\left[ctg^4\theta + ctg^2\theta - \frac{\sin4\varphi}{4} + \frac{1}{2}\right] - (\lambda_1-\lambda_2)\times\left[ctg^2\theta+\frac{1}{2}\right](\sin2\varphi-\cos2\varphi) - \lambda_3\cos^2 2\varphi\right\}\right\}$$

$$I_0(\theta,\varphi) = -k^6c^6\lambda_1\lambda_2\lambda_3\sin^4\theta\cos^2\theta,$$

$$\lambda_1 = \bar{A}^2\frac{\partial^2\varepsilon}{\partial\bar{A}^2}/c^2,\quad \lambda_2 = \bar{B}^2\frac{\partial^2\varepsilon}{\partial\bar{B}^2}/c^2,$$
$$\lambda_3 = p^2\frac{\partial^2\varepsilon}{\partial p^2}/c^2.\qquad c^2 = \partial P/\partial\rho.$$

Solving Eq. (8) we obtain three solutions corresponding to three sound branches of oscillations with sound velocity: $c_1(\theta,\varphi)$, $c_2(\theta,\varphi)$, $c_3(\theta,\varphi)$. The computer simulation clarifies the character of the anisotropy of spectra. In Fig. 1, the non-dimensional sound speeds $\tilde{c}_i = c_i(\theta,\varphi)/c$ $i=1,2,3$ are given.

Comparing the obtained results to the results presented in Refs. [4–6], it should be noted that in the latter, the additional modes related to the broken symmetry with respect to rotations in the configuration space are of dissipative character where the reactive component is absent. The accounting for the shape factor in the hydrodynamic equations for biaxial nematic crystals results in the reactive component being in the sound spectrum that is already under adiabatic approximation.

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