

On the acoustic approximation of thermomechanical model of a liquid crystal

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Abstract

Based on the equations of dynamics of a structurally inhomogeneous elastic medium taking into account the rotational degrees of freedom of the particles of microstructure, a simplified mathematical model is worked out for description of the wave motion in nematic liquid crystals under the influence of weak mechanical and thermal perturbations. It is shown that in the case of plane strain the shear stress in such a medium satisfies the Klein–Gordon equation, describing the oscillatory nature of particles rotation. The results of numerical computations shows that the natural frequency of rotational motion of the particles, determined by this equation, is the resonance characteristic of a material, and it is independent of the size of a sample and of the loading conditions.

1 Introduction

Liquid crystals have a wide range of applications due to the unusual combination of properties of fluidity and elastic anisotropy, which appear in a certain temperature range under weak external effects of different physical nature (mechanical, thermal, electrical, magnetic, optical). Such materials are used in the optical instruments, in the recording devices, displays, in the devices of processing and storage of information, in the medical and technical diagnostics, particularly in the thermography.

One of the common approaches to constructing mathematical models of liquid crystals is based on the representation of a crystal as a finely dispersed continuum, at each point of which the elongated particles (domains of oriented molecules) can move in accordance with the laws of dynamics of viscous or inviscid fluid and can rotate, encountering elastic or viscoelastic resistance to rotation. The fundamental work by the Cosserat brothers [1], where the equations of moment elastic continuum were written, has served the methodological basis of this approach. The model of a liquid crystal was firstly proposed by Eriksen [2] and developed by Aero, Bulygin, Kuvshinsky [3, 4], Leslie [5], as well as in more recent works by Kalugin [6], Kondaurov [7] and many others. In [8] the systems of nonlinear equations of the model of the Cosserat elastic continuum and of the reduced model, taking into account rotational degrees of freedom under vanishing couple stresses, are reduced to a thermodynamically consistent form of conservation laws that guarantee the mathematical correctness of the boundary–value problems for these systems.

This paper is devoted to the construction of a simplified model of a liquid crystal as an acoustic microinhomogeneous medium with rotating particles, based on the assumption of the dependence of potential energy of elastic deformation on the volume change, the angle of relative rotation of particles and the entropy. In the expression for inertia tensor the instantaneous orientation of the molecules of a liquid crystal is taken into account. The

thermal conductivity tensor in a medium describes the anisotropy, caused by the difference of coefficients of thermal conductivity in the direction along the axis of orientation of molecules and in the transverse direction.

2 Governing equations

Translational motion of a structurally heterogeneous material with rotating particles is described by the usual equation $x = \xi + u(\xi, t)$, which relates the Lagrange and Euler vectors of the center of mass of a particle by means of the displacement vector u . As a measure of deformation let us consider the tensor $\Lambda = R^* \cdot x_\xi$, where R is the orthogonal tensor of rotational motion of a particle, x_ξ is the tensor of distortion. Asterisk is used here to denote the operation of conjugation. Antisymmetric tensor of angular velocity of a particle is calculated by the formula $\Omega = \dot{R} \cdot R^*$.

The tensor of distortion can be written as a product of orthogonal and symmetric tensors: $x_\xi = R_e \cdot V$. Here R_e is the tensor of translational rotation and V is the Cauchy–Green measure of deformation. In the case of weak perturbations, when the displacement gradients are small, the approximation

$$R_e \approx I + \frac{u_x - u_x^*}{2}, \quad V \approx I + \frac{u_x + u_x^*}{2} \quad (1)$$

holds, where I is a unit tensor. Relative rotation of a particle is described by the orthogonal tensor R_r , which satisfies the equations $R = R_e \cdot R_r$ and $\Lambda = R_r^* \cdot V$. According to the first of these equations, rotational motion is a superposition of relative and translational rotations. The second one means that the chosen measure of deformation describes simultaneously two factors, which affect to the internal energy, namely the deformation of a medium and the relative rotation of particles.

In a Cartesian coordinate system the tensor Ω is identified with the vector of angular velocity $\omega = (\omega_1, \omega_2, \omega_3)$. The orthogonal tensor R_r can be represented as

$$R_r = I + \sin \phi Q + (1 - \cos \phi) Q^2, \quad (2)$$

where Q is an antisymmetric tensor associated with the unit vector $q = (q_1, q_2, q_3)$, ϕ is the angle of relative rotation of the particles, which is determined via the trace of R_r by the formula $\cos \phi = (\text{tr } R_r - 1)/2$. Vector q satisfies the equation $R_r \cdot q = q$, which means that it defines the direction of instantaneous relative axis of rotation.

The angular velocity tensor under the approximation (1) equals $\Omega = \dot{R}_e + \dot{R}_r \cdot R_r^*$. Omitting the details of computation of the product $\dot{R}_r \cdot R_r^*$, in which the auxiliary equalities $Q^3 = -Q$, $Q^4 = -Q^2$ and $Q \cdot \dot{Q} \cdot Q = 0$ are essentially used, let us give the final result:

$$\Omega = \frac{v_x - v_x^*}{2} + \dot{\phi} Q + \sin \phi \dot{Q} + (1 - \cos \phi) (Q \cdot \dot{Q} - \dot{Q} \cdot Q), \quad (3)$$

where v is the velocity vector of translational motion. Hence, after simple reduction, one can obtain the equation for the angle of relative rotation:

$$\dot{\phi} = \left(\omega_1 - \frac{v_{3,2} - v_{2,3}}{2} \right) q_1 + \left(\omega_2 - \frac{v_{1,3} - v_{3,1}}{2} \right) q_2 + \left(\omega_3 - \frac{v_{2,1} - v_{1,2}}{2} \right) q_3. \quad (4)$$

The governing equations of the model are derived from the integral laws of conservation of momentum, angular momentum and energy. For continuous motions with small

displacement gradients the Eulerian and Lagrangian variables are identified. In this case the integral conservation laws are equivalent to differential equations:

$$\rho_0 \dot{v} = \operatorname{div} \sigma + f, \quad \frac{\partial}{\partial t}(J \cdot \omega) = 2 \sigma^a + g, \quad \dot{W} = \sigma^* : (v_x - \Omega) - \operatorname{div} h + H, \quad (5)$$

where σ^a is the vector associated with the antisymmetric part of stress tensor and the colon means a double convolution of tensors, the rest notations are common. The inertia tensor J varies in time according to the equation $J = R \cdot J_0 \cdot R^*$, which can be justified by the transition to co-coordinate system associated with a rotating particle. The time derivative leads to the equation that is used, for example, in [7]:

$$\dot{J} = \dot{R} \cdot J_0 \cdot R^* + R \cdot J_0 \cdot \dot{R}^* = \Omega \cdot J - J \cdot \Omega. \quad (6)$$

Let us assume that thermodynamic state of a liquid crystal is determined by three parameters – the volume strain $\theta = \operatorname{div} u = \operatorname{tr} u_x$, the relative rotation angle ϕ and the entropy S . Then the last equation of (5), characterizing the change in the internal energy, gives the equation of balance of the power of elastic deformation

$$\begin{aligned} \frac{\partial W}{\partial \theta} \operatorname{tr} v_x + \frac{\partial W}{\partial \phi} \dot{\phi} &= \sigma^* : (v_x - \Omega) = \\ &= \sigma^* : \left(\frac{v_x + v_x^*}{2} - \dot{\phi} Q \right) - \sin \phi \sigma^* : \dot{Q} - (1 - \cos \phi) \sigma^* : (Q \cdot \dot{Q} - \dot{Q} \cdot Q), \end{aligned} \quad (7)$$

and the equation of heat transfer $T \dot{S} = -\operatorname{div} h + H$, where $T = \partial W / \partial S$ is the absolute temperature.

Taking into account that thermodynamic parameters of the state are functionally independent, from the first equation follows the system of constitutive relationships:

$$\begin{aligned} \operatorname{diag} \sigma &= \frac{\partial W}{\partial \theta} I, \quad \sigma - \operatorname{diag} \sigma = -(\sigma - \operatorname{diag} \sigma)^*, \\ \sigma^* : Q &= -\frac{\partial W}{\partial \phi}, \quad \sin \phi \sigma^* : \dot{Q} - (1 - \cos \phi) \sigma^* : (Q \cdot \dot{Q} - \dot{Q} \cdot Q) = 0. \end{aligned} \quad (8)$$

The last equation of (8) is a consequence of the independence of internal energy on the direction of axis of relative rotation. This ratio is reduced to the linear equation

$$A_1 \dot{q}_1 + A_2 \dot{q}_2 + A_3 \dot{q}_3 = 0 \quad (9)$$

with the coefficients

$$A_{s_1} = \sin \phi (\sigma_{s_3 s_2} - \sigma_{s_2 s_3}) - (1 - \cos \phi) \left((\sigma_{s_2 s_1} - \sigma_{s_1 s_2}) q_{s_2} - (\sigma_{s_1 s_3} - \sigma_{s_3 s_1}) q_{s_3} \right), \quad (10)$$

where (s_1, s_2, s_3) is an even permutation of indices. Variable quantities $(\dot{q}_1, \dot{q}_2, \dot{q}_3)$ in (9) are interrelated by means of the obvious condition $q_1 \dot{q}_1 + q_2 \dot{q}_2 + q_3 \dot{q}_3 = 0$. By the Lagrange rule $A_s = \lambda q_s$ ($s = 1, 2, 3$), where λ is the undetermined multiplier. These formulas restrict the general form of the stress tensor. The rest constitutive relationships give:

$$\sigma = -p I + \tau Q = \begin{pmatrix} -p & -\tau q_3 & \tau q_2 \\ \tau q_3 & -p & -\tau q_1 \\ -\tau q_2 & \tau q_1 & -p \end{pmatrix}, \quad p = -\frac{\partial W}{\partial \theta}, \quad \tau = -\frac{1}{2} \frac{\partial W}{\partial \phi}. \quad (11)$$

Concretizing the equation of state (11), let us take the following expression for internal energy: $W = k \theta^2 / 2 + \beta T_0 \theta + c_0 T + 2 \alpha \phi^2$, $S = \beta \theta + c_0 \ln(T/T_0)$. Here k is the bulk

modulus, α is the modulus of elastic resistance of a medium to rotation of the particles, β is the coefficient of thermal expansion, T_0 is the initial temperature, c_0 is the specific heat capacity per a unit volume. In this case the hydrostatic pressure p satisfies the Duhamel–Neumann equation: $p = -k\theta + \beta(T - T_0)$, and the tangential stress τ satisfies the Cosserat equation: $\tau = 2\alpha\phi$. Besides, the left side of the equation of heat transfer takes the form: $T\dot{S} = c_0\dot{T}$.

There is a simple way to calculate the vector q , included in the formula (4) for angle of relative rotation and in the representation (11) for the stress tensor, by introducing the vector–director n , oriented along the molecules of a liquid crystal. The rotation of this vector is described by the tensor R , therefore $n = R \cdot n^0$, $\dot{n} = \dot{R} \cdot n^0$, $\dot{n} = \Omega \cdot n$, where n^0 is the initial position of the vector n . Since under the assumptions of small displacement gradients the tensor of translational rotation is identified with a unit tensor, then $q = n^0 \times n / |n^0 \times n|$.

A direct calculation of the inertia tensor for an ensemble of oriented particles via the vector–director by well-known formulas of the classical solid mechanics gives:

$$J = j_0 \begin{pmatrix} 1 - n_1^2 & -n_1 n_2 & -n_1 n_3 \\ -n_1 n_2 & 1 - n_2^2 & -n_2 n_3 \\ -n_1 n_3 & -n_2 n_3 & 1 - n_3^2 \end{pmatrix}, \quad (12)$$

where j_0 is the product of the moment of inertia of a single particle and the number of particles in a unit volume. It is easy to check that this tensor satisfies (6).

If \varkappa and \varkappa' are coefficients of thermal conductivity in the direction of orientation of molecules and in the transverse direction, then the thermal conductivity tensor is

$$K = \varkappa' \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + (\varkappa - \varkappa') \begin{pmatrix} n_1^2 & n_1 n_2 & n_1 n_3 \\ n_1 n_2 & n_2^2 & n_2 n_3 \\ n_1 n_3 & n_2 n_3 & n_3^2 \end{pmatrix}. \quad (13)$$

According to the Fourier law, $h = -K \cdot \text{grad } T$.

Assuming that the internal heat production depends on rotation of the particles, the following expression for $H = \gamma\omega^2$ can be taken, where γ is the empirical coefficient of viscosity of a medium.

A complete system of equations of simplified mathematical model in expanded form consists of the equations of translational and rotational motion

$$\begin{aligned} \rho_0 \dot{v}_1 &= -p_{,1} - (\tau q_3)_{,2} + (\tau q_2)_{,3} + f_1, \\ \rho_0 \dot{v}_2 &= -p_{,2} + (\tau q_3)_{,1} - (\tau q_1)_{,3} + f_2, \\ \rho_0 \dot{v}_3 &= -p_{,3} - (\tau q_2)_{,1} + (\tau q_1)_{,2} + f_3, \\ \frac{\partial}{\partial t} (J_{s1} \omega_1 + J_{s2} \omega_2 + J_{s3} \omega_3) &= 2\tau q_s + g_s, \end{aligned} \quad (14)$$

the equations of state

$$\begin{aligned} \dot{p} &= -k(v_{1,1} + v_{2,2} + v_{3,3}) + \beta\dot{T}, \\ \dot{\tau} &= \alpha(v_{3,2} - v_{2,3} - 2\omega_1)q_1 + \alpha(v_{1,3} - v_{3,1} - 2\omega_2)q_2 + \alpha(v_{2,1} - v_{1,2} - 2\omega_3)q_3, \end{aligned} \quad (15)$$

the thermal conductivity equation

$$c_0 \dot{T} = -h_{1,1} - h_{1,1} - h_{1,1} - \beta T(v_{1,1} + v_{2,2} + v_{3,3}) + \gamma(\omega_1^2 + \omega_2^2 + \omega_3^2) \quad (16)$$

and the equation for the vector–director

$$\dot{n}_1 = -\omega_3 n_2 + \omega_2 n_3, \quad \dot{n}_2 = \omega_3 n_1 - \omega_1 n_3, \quad \dot{n}_3 = -\omega_2 n_1 + \omega_1 n_2. \quad (17)$$

Here $h_s = -K_{s1}T_{,1} - K_{s2}T_{,2} - K_{s3}T_{,3}$. Components of the inertia tensor and of the thermal conductivity tensor are given by the formulas (12) and (13).

3 Plane case

The equations of plane motion are simplified, because the vector–director can be easily calculated by the absolute angle φ of rotation of the molecules of a liquid crystal, and the vector q , that specifies the axis of relative rotation, coincides with a unit coordinate vector, orthogonal to the plane of motion. Governing system of the equations can be written as follows:

$$\begin{aligned} \rho_0 \frac{\partial v_1}{\partial t} &= -\frac{\partial p}{\partial x_1} - \frac{\partial \tau}{\partial x_2} + f_1, & \rho_0 \frac{\partial v_2}{\partial t} &= \frac{\partial \tau}{\partial x_1} - \frac{\partial p}{\partial x_2} + f_2, & j_0 \frac{\partial \omega}{\partial t} &= 2\tau + g, \\ \frac{\partial p}{\partial t} &= -k \left(\frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} \right) + \beta \frac{\partial T}{\partial t}, & \frac{\partial \tau}{\partial t} &= \alpha \left(\frac{\partial v_2}{\partial x_1} - \frac{\partial v_1}{\partial x_2} \right) - 2\alpha \omega, \\ c_0 \frac{\partial T}{\partial t} &= \frac{\partial}{\partial x_1} \left((\varkappa \cos^2 \varphi + \varkappa' \sin^2 \varphi) \frac{\partial T}{\partial x_1} + (\varkappa - \varkappa') \sin \varphi \cos \varphi \frac{\partial T}{\partial x_2} \right) + \\ &+ \frac{\partial}{\partial x_2} \left((\varkappa - \varkappa') \sin \varphi \cos \varphi \frac{\partial T}{\partial x_1} + (\varkappa \sin^2 \varphi + \varkappa' \cos^2 \varphi) \frac{\partial T}{\partial x_2} \right) - \\ &- \beta T \left(\frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} \right) + \gamma \omega^2, & \frac{\partial \varphi}{\partial t} &= \omega. \end{aligned} \quad (18)$$

In general case by differentiation of the system (18) one can obtain the Klein–Gordon equation for tangential stress (Δ is the two-dimensional Laplace operator):

$$\frac{\partial^2 \tau}{\partial t^2} = \frac{\alpha}{\rho_0} \Delta \tau - \frac{4\alpha}{j_0} \tau + r, \quad r = \frac{\alpha}{\rho_0} \left(\frac{\partial f_2}{\partial x_1} - \frac{\partial f_1}{\partial x_2} \right) - \frac{2\alpha}{j_0} g. \quad (19)$$

The homogeneous Klein–Gordon equation describes oscillatory solutions with the period $t_* = \pi \sqrt{j_0/\alpha}$ and the cyclic frequency $\nu_* = 1/t_*$, which are independent on the spatial coordinates. Waves of rotational motion in the Cosserat elastic continuum have the same period and frequency. It is a resonant frequency [8], which is the characteristic of a material independent on the size of a sample and the loading conditions. In the absence of body forces and moments the equation (19) describes a propagation of monochromatic waves $\tau = \hat{\tau} \exp i(2\pi\nu t - l \cdot x)$ with dispersion. Dispersion equation, which relates the scalar square of the wave vector l with the frequency ν , has the form: $l^2 = 4\pi^2 \rho_0 (\nu^2 - \nu_*^2)/\alpha$. The phase velocity of waves takes the real value $a = 2\pi\nu/|l|$ only for high-frequency waves with $\nu \geq \nu_*$. If $\nu \rightarrow \infty$, then a goes to the velocity $a_\infty = \sqrt{\alpha/\rho}$ of transverse waves, and if $\nu \rightarrow \nu_*$, then a goes to zero. Low-frequency waves with $\nu < \nu_*$ are the exponentially damped standing waves, the damping rate of which is equal to $1/|l|$.

4 Numerical results

After the transition to dimensionless variables $t \mapsto 2t\sqrt{\alpha/j_0}$ and $x \mapsto 2x\sqrt{\rho_0/j_0}$ the equation (19) leads to the Klein–Gordon equation with unit coefficients. This equation was solved numerically by means of a finite-difference scheme “cross” in a rectangle with

the side $b = 50$. The value for side of a rectangle was selected taking into account the fact, that linear scale in dimensionless equation is the characteristic size of particles in the microstructure of a material. Computations were performed on two difference grids, composed of 500×500 and 1000×1000 nodes. Comparison of the results showed a good agreement.

In Fig. 1 one can see the surfaces of tangential stress, corresponding to the dimensionless time $t = 20\pi$, for the problem about the action of the localized volume moments $g = g_0 \sin(1.5\pi t)$ (Fig. 1 *a*) and $g = g_0 \sin(2\pi t)$ (Fig. 1 *b*) at zero stresses on both horizontal boundaries.

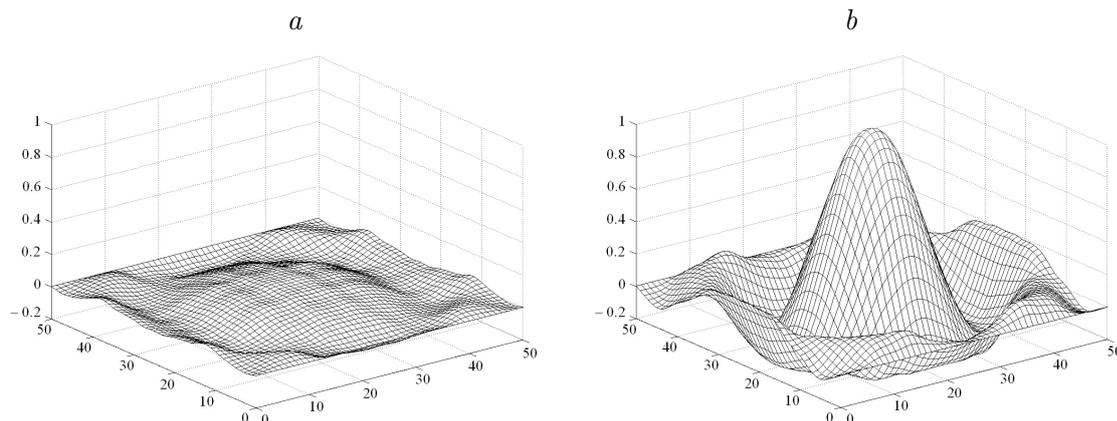


Figure 1: Non-resonant (*a*) and resonant (*b*) loading by localized moment

In Fig. 2 the volume moment is zero, and a uniformly distributed tangential stress acts on the part of a boundary, which varies with time according to the periodic law: $\tau = \tau_0 \sin(1.5\pi t)$ (Fig. 2 *a*), $\tau = \tau_0 \sin(2\pi t)$ (Fig. 2 *b*).

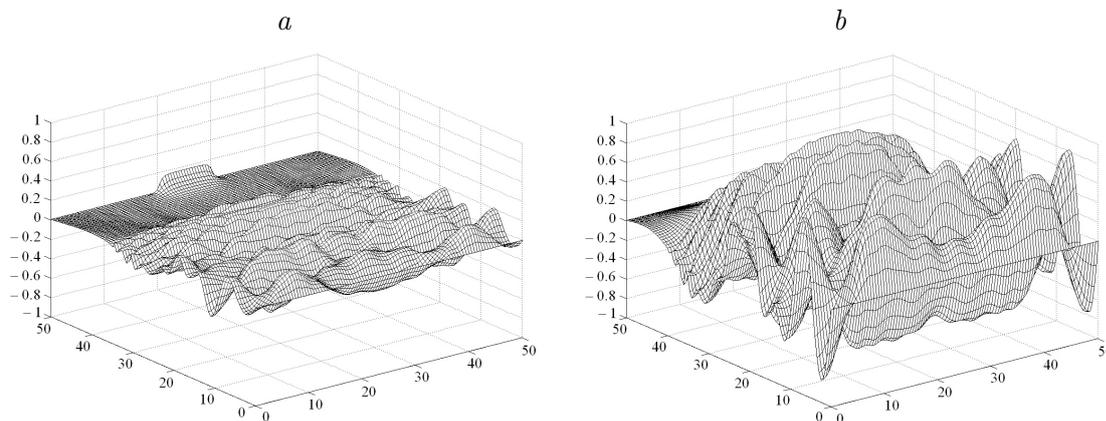


Figure 2: Non-resonant (*a*) and resonant (*b*) loading by tangential stress

In both Figures the maximum of amplitude of tangential stress is equal to one due to the choice of g_0 and τ_0 . Computations show that the dimensionless frequency $\nu_* = 1$ is the resonant frequency for a liquid crystal. This is expressed in significantly greater amplitudes of tangential stress in Figs. 1 *b* and 2 *b* as compared with Figs. 1 *a* and 2 *a*, where the excitation frequency ν is lower than the resonant frequency. A similar ratio for the amplitudes takes place, when $\nu > \nu_*$.

The equation (19) shows that if a liquid crystal is in the natural state at initial time

moment under the neglecting body forces and moments and if the tangential stress, which completely determines the rotational motion of particles, is equal to zero on the boundary, then it remains zero at any time moment in all interior points of a crystal. It also follows that the temperature influences on rotations of the particles in the system (18) only through the boundary conditions of the problem. This means that the change of orientation of the liquid crystal molecules is impossible by means of the thermal action on the stress-free boundary of a medium. So, the effect of orientational thermoelasticity of a nematic liquid crystal, which is discussed in [9], is connected with the appearance of tangential stresses on the boundary.

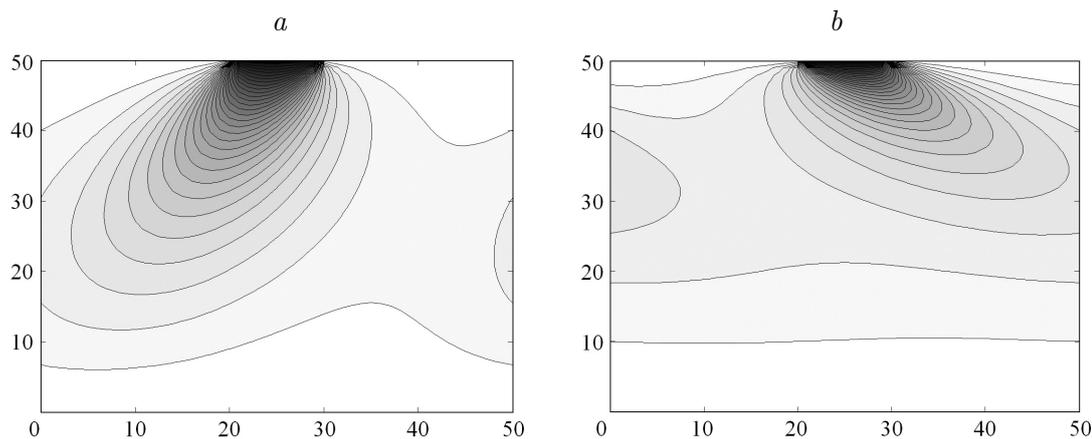


Figure 3: Level curves of the temperature at different ratios between the coefficients of thermal conductivity α and α' in the direction of orientation of molecules and in the opposite direction: $\alpha = 5 \alpha'$ (a), $\alpha = \alpha'/5$ (b)

Computational results of the stationary temperature field in a liquid crystal, the particles of which are oriented at the angle 60° , are represented in Fig. 3 for the cases when $\alpha = 5 \alpha'$ (Fig. 3 a) and $\alpha = \alpha'/5$ (Fig. 3 b). The initial temperature field is considered to be homogeneous, a constant temperature distribution is given on a part of the upper boundary of computational domain, conditions of periodicity are taken on the lateral boundaries.

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