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GENERAL ANALYSIS OF LINEAR NEMATIC ELASTICITY

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The results of a general analysis of linear nematic elasticity on the basis of the five-parameter thermodynamic potential of de Gennes (DG) have been presented. It has been shown that, depending on the similarity of the material parameters to the conditions of marginal (limiting) stability, the DG potential describes the entire diversity of soft, semisoft, and harder behavior of weakly elastic nematic solids. It has been established that an additional soft mode of longitudinal stretching, acting along the director, can also exist alongside the known shear soft modes. A theorem on the special rotational invariance of the stress-tensor components, which is close to the principle of rotational invariance postulated earlier by Olmsted, has been proved. It has been shown that the stress tensor is symmetric if the shear modes are soft. In this case, the reduced DG potential is reduced to a one-parameter nematic potential. If the mode of longitudinal stretching is also soft, this dimensionless parameter contains no additional parameters. Simple shear and simple tension have been considered as an illustration of the theory elaborated.

Introduction. Different continuous theories including internal rotations in force energy were proposed to describe the anisotropic elasticity of liquid-crystalline elastomers. Employing simple symmetry considerations, de Gennes [1] was the first to introduce internal rotations into the density of free energy for nematic elastomers (see also [2]). Different effects in nematic elastomers and gels have recently been studied at a phenomenological level by many researchers [3–10]. Several molecular theories have also been developed [11–19].

Soft modes in nematic elastomers were described for the first time by Warner et al. [19]. Golubovich and Lubenskii [20] had earlier predicted the existence of soft modes for certain solid bodies with internal degrees of freedom on symmetry grounds. Soft elasticity reflects the deformability of multidomain nematics without expending elastic energy. Theoretical predictions of this striking effect with the use of the de Gennes and Warner potentials were later confirmed experimentally (see, for example, [17]). In [21], Lubenskii et al. attempted to consider all the previous results on symmetry grounds and on the basis of the standard approaches of continuum mechanics.

Despite the above-mentioned success of the theory, general conditions for the appearance of soft modes have not been established. One mainly employs the Warner potential, which always predicts only soft (shear) modes. Therefore, soft elasticity must generally be analyzed based on a more general potential, for example, such as the de Gennes potential, in the linear case. The principle of rotational invariance, employed in the literature to substantiate the existence of soft modes, has been postulated; therefore, it needs explanation itself.

In the present work, we propose a general approach that simplifies an analysis of this problem. Unlike the principle of rotational invariance, this approach allows general classification of the behavior of nematic solid bodies as hard, semisoft, and soft behavior. A new soft/semisoft mode of longitudinal stretching has been found.

Alongside the nematic elastomers, there are other polymer nematics which demonstrate semisoft or even harder behavior. The nonlinear potential of Warner, even in the linear limit, cannot describe these polymers. Therefore, it is of interest to comprehensively analyze linear nematic elasticity within the framework of the more general de Gennes potential [1]. This is the prime objective of the present work. The authors also hope that their results will enable

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one to include the theory of linear nematic elasticity of liquid-crystalline elastomers in the general structure of the mechanics of a rigid body with a strictness level accepted in this field.

1. Kinematics, Free Energy, and Stresses. For elastic solid bodies of the nematic type, the kinematic relation between the initial value of the director in an undeformed state $\underline{n}$ and its value in a deformed state $\underline{n}_{\rm d}$ has the form of an orthogonal transformation

$$\underline{n}_{\rm d} = \underline{\underline{R}}\cdot\underline{n}\,, \quad \underline{\underline{R}} = \exp\left(-\underline{\underline{\omega}}^{\rm I}\right) \tag{1}$$

with orthogonal tensor $\underline{\underline{R}}$. Here $\underline{\underline{\omega}}^{\rm I}$ is the antisymmetric tensor of finite internal rotations, which is related to the vector of internal rotation $\underline{\omega}^{\rm I}$ by the relation $\omega^{\rm I}_{ik} = -\delta_{ijk}\omega^{\rm I}_j$. In the linear case where the internal rotations are fairly small, Eq. (1) is reduced to the form

$$\underline{n}_{\rm d} - \underline{n} \approx -\underline{\underline{\omega}}^{\rm I}\cdot\underline{n} = \underline{\omega}^{\rm I}\times\underline{n}\,, \quad \left|\underline{\underline{\omega}}^{\rm I}\right| = \left|\underline{\omega}^{\rm I}\right| << 1\,. \tag{2}$$

For nematic solid bodies, Eqs. (1) and (2) are supplemented with the well-known equations of the dynamics of internal rotations (see, for example, [22, 23]) and the expression for free energy.

Thermodynamic state variables are represented in this theory by the tensors of infinitesimal deformations $\underline{\underline{e}}$ and relative rotations $\underline{\underline{\omega}} = \underline{\underline{\omega}}^{\rm B} - \underline{\underline{\omega}}^{\rm I}$. Here $\underline{\underline{\omega}}^{\rm B}$ is the tensor of rotation of the entire element of a medium. The tensors $\underline{\underline{e}}$ and $\underline{\underline{\omega}}^{\rm B}$ are expressed by the displacement vector $\underline{u}$ with the use of the ordinary linear-elasticity formulas: $2\underline{\underline{e}} = \nabla\underline{u} + (\nabla\underline{u})^{\rm T}$ and $2\underline{\underline{\omega}}^{\rm B} = \nabla\underline{u} - (\nabla\underline{u})^{\rm T}$. To simplify the analysis in what follows we consider the incompressible case $\mathrm{tr}\,\underline{\underline{e}} = 0$. Orientation of the medium in an undeformed state is described by the unit vector (director) $\underline{n}$.

Employing simple invariance considerations, de Gennes [1] introduced the potential which describes nematic linear elasticity with the use of the deformation part of the free energy f determined in the form

$$2f = \mu_0\,(\underline{n}\underline{n} : \underline{\underline{e}})^2 + \mu_1\,(\underline{n}\times\underline{\underline{e}}\times\underline{n})^2 + \mu_2\,(\underline{n}\times\underline{\underline{e}}\times\underline{n})^2 + \alpha_1\,(\underline{\omega}\times\underline{n})^2 + \alpha_2\underline{n}\cdot\underline{\underline{e}}\cdot\underline{\omega}\times\underline{n}\,. \tag{3}$$

Here μ_k and α_k are five material parameters with the dimensions of elastic moduli. Using the formulas

$$(\underline{n}\times\underline{\underline{e}}\times\underline{n})_s = \delta_{ejk}n_j e_{ke} n_m \delta_{mes}\,, \quad (\underline{n}\cdot\underline{\underline{e}}\times\underline{n})_s = n_k e_{kt} n_m \delta_{mts}$$

we reduce Eq. (3) to the form

$$f = \frac{1}{2}G_0\,\left|\underline{\underline{e}}\right|^2 + G_1\underline{n}\,\underline{n} : \underline{\underline{e}}^2 + G_2\,(\underline{n}\,\underline{n} : \underline{\underline{e}})^2 - 2G_3\underline{n}\,\underline{n} : (\underline{\underline{e}}\cdot\underline{\underline{\omega}}) - G_4\underline{n}\,\underline{n} : \underline{\underline{\omega}}^2\,, \tag{4}$$

which is more convenient for our analysis. This expression represents the expansion of free energy in irreducible basis tensor invariants. In it, use has been made of the following notation:

$$G_0 = \mu_1\,, \quad G_1 = \frac{1}{2}\mu_2 - \mu_1\,, \quad G_2 = \frac{1}{2}(\mu_0 + \mu_1 - \mu_2)\,, \quad G_3 = \frac{1}{4}\alpha_2\,, \quad G_4 = \frac{1}{2}\alpha_1\,. \tag{5}$$

The material constants in (4) depend on the scalar parameter of order Q_0 in an undeformed state. In transition to an isotropic state, the "nematic" moduli G_k (k = 1, 2, 3, 4) vanish. The "isotropic" modulus G_0 remains nonzero. In a deformed state, the value of the scalar order parameter Q can be different from Q_0. According to [24], we have $Q - Q_0 \sim (\underline{n}\,\underline{n}{:}\underline{\underline{e}})^2$ for the change in the scalar order parameter under deformation. Thus, this effect is already described by the parameter G_2 in (4).

The constitutive equations for the symmetric $\underline{\underline{\sigma}}^{\rm s}$ and antisymmetric $\underline{\underline{\sigma}}^{\rm a}$ parts of the extra (excess)-stress tensor computed with the use of the expression for the free energy of de Gennes (4) have the form

$$\underline{\underline{\sigma}}^{s} = \frac{\partial f}{\partial \underline{\underline{e}}} = G_0 \underline{\underline{e}} + G_1 \left(\underline{n}\,\underline{n}\cdot\underline{\underline{e}} + \underline{\underline{e}}\cdot\underline{n}\,\underline{n}\right) + 2G_2 \underline{n}\,\underline{n}\left(\underline{\underline{e}} : \underline{n}\,\underline{n}\right) + G_3 \left(\underline{n}\,\underline{n}\cdot\underline{\underline{\omega}} - \underline{\underline{\omega}}\cdot\underline{n}\,\underline{n}\right) , \tag{6a}$$

$$\underline{\underline{\sigma}}^{a} = \frac{\partial f}{\partial \underline{\underline{\omega}}} = G_3 \left(\underline{n}\,\underline{n}\cdot\underline{\underline{e}} - \underline{\underline{e}}\cdot\underline{n}\,\underline{n}\right) + G_4 \left(\underline{n}\,\underline{n}\cdot\underline{\underline{\omega}} + \underline{\underline{\omega}}\cdot\underline{n}\,\underline{n}\right) . \tag{6b}$$

The total stress tensor can be written in the form $\underline{\underline{\sigma}} = -p\underline{\underline{\delta}} + \underline{\underline{\sigma}}^{s} + \underline{\underline{\sigma}}^{s}$.

The material parameters G_k ("moduli") in (4) represent scale factors for independent basis tensor invariants. Therefore, in what follows we employ the following conditions:

$$G_k \neq 0 \quad (k = 0, 1, 2, 3, 4) , \tag{7}$$

to exclude degeneration of Eqs. (4) and (6).

To take account of the smallness of deformations and internal rotations in comparing the order of the values of different variables in the general case we can take

$$|\underline{\underline{e}}| \sim |\underline{\underline{\omega}}| \sim \varepsilon < \ 0 < \varepsilon << 1 . \tag{8}$$

Next we employ the kinematic and dynamic variables normalized on the basis of the parameter ε as follows:

$$\underline{\underline{e}} \rightarrow \underline{\underline{e}}/\varepsilon , \quad \underline{\underline{\omega}} \rightarrow \underline{\underline{\omega}}/\varepsilon , \quad \underline{\underline{\sigma}} \rightarrow \underline{\underline{\sigma}}/\varepsilon , \quad f \rightarrow f/\varepsilon^2 . \tag{9}$$

To simplify the analysis we introduce a special (local) Cartesian coordinate system $\{\underline{\hat{x}}\}$ whose one axis $\hat{x}_1$ is guided along the initial director $\underline{n}$. In this coordinate system $\{\underline{\hat{x}}\}$, where $\underline{n} = \{1, 0, 0\}$, the free energy (4) takes the form

$$\hat{f} = \left(\frac{1}{2} G_0 + G_1 + G_2\right)\hat{e}_{11}^{\,2} + \frac{1}{2} G_0 \left(\hat{e}_{22}^{\,2} + \hat{e}_{33}^{\,2} + 2\hat{e}_{23}^{\,2}\right) + \sum_{k=2,3} \left[(G_0 + G_1)\, \hat{e}_{1k}^{\,2} + 2G_3 \hat{\omega}_{1k} \hat{e}_{1k} + G_4 \hat{\omega}_{1k}^{\,2}\right] . \tag{10}$$

In what follows, all the tensor components in $\{\underline{\hat{x}}\}$, normalized according to (9), are marked by upper caps (for example, $\hat{f}$). Because of the incompressibility condition, not all the terms in (10) are independent. Employing this condition, for example, in the form $\hat{e}_{33} = -(\hat{e}_{11} + \hat{e}_{22})$, we obtain the equivalent expression for free energy

$$\hat{f} = \left(\frac{3}{4} G_0 + G_1 + G_2\right)\hat{e}_{11}^{\,2} + G_0 \left[\left(\hat{e}_{22} + \frac{1}{2}\hat{e}_{11}\right)^2 + \hat{e}_{23}^{\,2}\right] + \sum_{k=2,3} \left[(G_0 + G_1)\, \hat{e}_{1k}^{\,2} + 2G_3 \hat{\omega}_{1k} \hat{e}_{1k} + G_4 \hat{\omega}_{1k}^{\,2}\right] . \tag{11}$$

which contains only independent terms.

The constitutive equations (6a) and (6b) written in the coordinate system $\{\underline{\hat{x}}\}$ and normalized according to (9) have the form

$$\hat{\sigma}_{11}^{s} = (G_0 + 2G_1 + 2G_2)\, \hat{e}_{11} , \quad \hat{\sigma}_{22}^{s} = G_0 \hat{e}_{22} , \quad \hat{\sigma}_{33}^{s} = G_0 \hat{e}_{33} , \quad \hat{\sigma}_{23}^{s} = G_0 \hat{e}_{23} , \tag{12a}$$

$$\hat{\sigma}_{1k}^{s} = (G_0 + G_1)\, \hat{e}_{1k} + G_3 \hat{\omega}_{1k} , \quad \hat{\sigma}_{1k}^{a} = G_3 \hat{e}_{1k} + G_4 \hat{\omega}_{1k} \quad (k = 2, 3) . \tag{12b}$$

Here the antisymmetric components of the stress tensor are presented only for $k < j$.

Each of the nine pairs $\{\hat{e}_{ij}, \hat{\omega}_{ij}\}$ of kinematic variables in (12) will be called the $\{i, j\}$ deformational/rotational mode or simply the $\{i, j\}$ mode. The modes in (12) with $i = j$ and $i \neq j$ are called normal and shear modes respectively.

In what follows, we will mainly consider the shear modes $\{1, k\}/\{k, 1\}$, which are denoted as $\{1, k\}$ for the sake of simplification, and the special stretching (elongation) mode $\{11 - 22\}$ corresponding to the deformation difference $\hat{e}_{11} - \hat{e}_{22}$.

The thermodynamic stability of the system imposes the conditions of being positive definite on expression (11) for free energy. Since all the terms in (11), including the last two quadratic forms for k = 2 and 3, are independent, the necessary and sufficient stability conditions have the form

$$G_0 > 0 , \quad G_4 > 0 , \quad G_0 + G_1 > 0 , \quad \frac{3}{4} G_0 + G_1 + G_2 > 0 , \quad (G_0 + G_1)\, G_4 > G_3^2 . \tag{13}$$

Formulas (5) enable us to rewrite inequalities (13) in terms of the material parameters appearing in (3):

$$\mu_0 + \frac{1}{2}\mu_1 > 0 , \quad \mu_1 > 0 , \quad \mu_2 > 0 , \quad 4\alpha_1\mu_2 > \alpha_2^2 \quad (\alpha_1 > 0) . \tag{14}$$

It should be noted that the first stability condition in (14) differs from the *sufficient* stability condition $\mu_0 > 0$ actually employed in [11] and [16]. This condition is obtained when all the terms in (10) are considered as being independent, i.e., the incompressibility condition is disregarded. The necessary and sufficient stability conditions (13) and (14) are critically important for determination of the conditions of marginal stability discussed below.

If the set of parameters $P = \{G_0, ..., G_4\}$ satisfies conditions (7) and (13), the relationships between the tensors $\underline{\underline{e}}$, $\underline{\underline{\omega}}$, and $\underline{\underline{\sigma}}$, described by the constitutive equations (6), are always unique. This fact is apparent for the constitutive relations (12a). It is also clear for relations (12b) if they are considered as two interrelated linear algebraic equations with the positive determinant

$$D \equiv (G_0 + G_1)\, G_4 - G_3^2 > 0 . \tag{15}$$

Quite apparently, this result, proved for the particular case (12) in the special coordinate system $\{\hat{x}\}$, holds for the constitutive equations written in general form in (6).

2. Marginal Stability and Soft and Semisoft Modes. Marginal stability develops when certain inequalities in (13) change to equalities. Because of the constraints (13), we can have only two conditions of marginal stability:

$$\frac{3}{4} G_0 + G_1 + G_2 = 0 , \tag{16}$$

$$D \equiv (G_0 + G_1)\, G_4 - G_3^2 = 0 . \tag{17}$$

The $\{i, j\}$ modes whose parameters satisfy relations (16) or (17) will be called marginally stable.

There can be cases where stability conditions (13) are fulfilled but the last two inequalities in (13) are close to conditions (16) and (17):

$$\frac{3}{4} G_0 + G_1 + G_2 = O\,(\delta) , \tag{18a}$$

$$D \equiv (G_0 + G_1)\, G_4 - G_3^2 = O\,(\delta) . \tag{18b}$$

Here we have $0 < \delta << 1$. Stable $\{i, j\}$ modes whose parameters P satisfy (18a) or (18b) will be called nearly marginally stable.

We determine the $\{i, j\}$ mode as being soft if the condition $\hat{\sigma}_{ij} = 0$ is fulfilled for the nontrivial deformations and relative rotations $\hat{e}_{ij}$ and $\hat{\omega}_{ij} = O_{ij}$ (1). The constitutive equations (12) show that soft modes, if any, are determined by the shear modes $\{1, k\}$ described by (12b) or by the special mode of longitudinal stretching $\{11 - 22\}$.

We consider first possible soft shear modes $\{1, k\}$ when $\hat{\sigma}_{1k} = \hat{\sigma}_{k1} = 0$. Owing to (17), we have unique relationships between the relative rotations and corresponding deformations in the soft shear modes $\{1, k\}$, although these deformations are not unique. Let us consider simple tension (stretching) along the $\hat{x}_1$ axis. In this case, the deformation tensor $\underline{\underline{e}}$ has the form $\underline{\underline{e}} = \varepsilon\cdot\underline{\underline{\mathrm{diag}}}\{1, -1/2, -1/2\}$, whereas the elongation stress $\hat{\sigma}_{\mathrm{el}} = \hat{\sigma}_{11} - \hat{\sigma}_{22}$ is determined, according to (12a), in the form

$$\hat{\sigma}_{\mathrm{el}} = \left(\frac{3}{2} G_0 + 2G_1 + 2G_2\right)\varepsilon . \tag{19}$$

Thus, if the mode of longitudinal stretching is soft, i.e., $\hat{\sigma}_{\mathrm{el}} = 0$ when $\varepsilon \neq 0$, Eq. (19) is reduced to the condition of marginal stability (16), and conversely. It is apparent that the modes described above make no contribution to the free energy. Consequently, if they exist, they lead to a minimum of the free energy in the parametric "space."

Semisoft modes are determined as stable $\{i, j\}$ modes in the constitutive equations (12) if the relations

$$\hat{\sigma}_{\mathrm{el}}/G_0 = O(\delta) \quad \text{and} \quad \hat{\sigma}_{1k}/G_3 = O(\delta) \quad \text{for} \quad \hat{e}_{ij}, \hat{\omega}_{ij} = O_{ij}(1) \tag{20}$$

hold for the positive small parameter δ. The stresses for semisoft modes and their contribution to the free energy are much lower than those for other modes. A nonlinear analysis of semisoft deformations on the basis of the potential of Warner et al. [17] has revealed good agreement with experimental data. However this analysis is beyond the scope of our consideration.

The general behavior of weakly elastic nematic solid bodies can now be formally classified in terms of the parameter δ as soft ($\delta = 0$), semisoft ($0 < \delta << 1$), and hard ($\delta > \sim 1$) behaviors.

Let us establish the relations between the conditions of existence of soft (or semisoft) modes (16) and (17) (or (18a) and (18b)) and Eqs. (12) and (19).

Equation (19) shows that the *mode of longitudinal stretching* $\{11 - 22\}$ *is soft (semisoft) if and only if it is marginally (or nearly marginally) stable*.

We can easily analyze soft (semisoft) nematic shearing modes $\{1, k\}$, employing the constitutive equations (12b). If the shear stresses vanish, i.e., $\hat{\sigma}^{\mathrm{s}}_{1k} = \hat{\sigma}^{\mathrm{a}}_{1k} = 0$, the nontrivial solution of the system of equations (12b) for $\hat{e}_{1k}$ and $\hat{\omega}_{1k}$ is existent if its determinant is equal to zero, $D = 0$, i.e., relation (17) holds. This means that the soft shear modes $\{1, k\}$ are marginally stable. If $D = 0$, the nontrivial solutions of system (12b) — $\hat{e}_{1k}$ and $\hat{\omega}_{1k}$ — are existent not only when $\hat{\sigma}^{\mathrm{s}}_{1k} = \hat{\sigma}^{\mathrm{a}}_{1k} = 0$ but also in the case $\hat{\sigma}^{\mathrm{s}}_{1k} \sim \hat{\sigma}^{\mathrm{a}}_{1k} \neq 0$. This means that marginally stable $\{1, k\}$ modes are not unique, and in this case we have hard marginally stable modes alongside the soft modes. As is seen from Eqs. (10) and (11), soft shear modes are physically more preferable since they are more profitable energetically. An elementary analysis shows that an analogous situation occurs for semisoft shear modes. Summing up these results, we arrive at the following conclusion: *soft (or semisoft)* $\{1, k\}$ *shear modes exist if and only if the condition of marginal (or nearly marginal) stability (17)* (or (18b)) *is fulfilled*.

3. Rotational Invariance and Nematic Modes. Up to this point, the Cartesian axes $\hat{x}_2$ and $\hat{x}_3$ have been assumed to be fixed in the $\{\hat{x}_2\hat{x}_3\}$ plane, which is orthogonal to the director. Let us consider the influence of rigid rotations of the $\hat{x}_2$ and $\hat{x}_3$ axes in the $\{\hat{x}_2\hat{x}_3\}$ plane of the behavior of stresses and soft and semisoft modes. The orthogonal matrix $\underline{\underline{q}}$ describing these plane rotations has the form

$$\underline{\underline{q}}(\alpha) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix}. \tag{21}$$

The stress tensor resulting from the rotation (21) will be denoted by $\underline{\underline{\hat{\sigma}}}' = \underline{\underline{q}}^{\mathrm{T}}\cdot\underline{\underline{\hat{\sigma}}}\cdot\underline{\underline{q}}$ and $\underline{\underline{\hat{\sigma}}}^{\mathrm{T}\prime} = \underline{\underline{q}}^{\mathrm{T}}\cdot\underline{\underline{\hat{\sigma}}}^{\mathrm{T}}\cdot\underline{\underline{q}}$. Computing the transformed components of the stress tensors $\hat{\sigma}'_{11}$, $\hat{\sigma}'_{1k}$, and $\hat{\sigma}'_{k1}$ (k = 2, 3), we obtain

$$\hat{\sigma}'_{11} = \hat{\sigma}_{11}, \quad \hat{\sigma}'_{12} = \hat{\sigma}_{12}\cos\alpha + \hat{\sigma}_{13}\sin\alpha, \quad \hat{\sigma}'_{13} = -\hat{\sigma}_{12}\sin\alpha + \hat{\sigma}_{13}\cos\alpha . \tag{22}$$

The same relations hold for $\hat{\sigma}'_{k1}$. These formulas show that if the modes $\{1, k\}$ are soft for particular positions of the $\hat{x}_2$ and $\hat{x}_3$ axes in the plane $\{\hat{x}_2\hat{x}_3\}$, i.e., $\{\hat{\sigma}_{1k}\} = 0$ (k = 2 and 3), they are soft for any Cartesian axes $\hat{x}'_2$ and $\hat{x}'_3$ located in the same plane. The shear stresses will be called *rotationally invariant* if they do not change their values in rotations described by matrix (21). Then formulas (22) show that the shear stresses are rotationally invariant for soft modes. Relations (22) for semisoft modes, where $\{\hat{\sigma}_{k1}\} = O$ (k = 2 and 3), show that semisoft modes are also rotationally invariant. It follows that the *set of soft (semisoft) shear modes has the power of a continuum*. This result, known earlier from [10] by Olmsted, is almost apparent for soft modes, since the $\hat{x}_2$ and $\hat{x}_3$ axes are located arbitrarily in the $\{\hat{x}_2\hat{x}_3\}$ plane. As is clear from the first relation of (22), the soft stretching mode $\{1, 1-12\}$ also remains soft (semisoft) in transformation of rotation with matrix (21).

We consider the inverse problem: under which condition are the components of the stress tensor $\hat{\sigma}_{ij}$ rotationally invariant? Here, too, of interest are only plane rotations about the director (about the $\hat{x}_1$ axis) which are described by matrix (21). In this case, formal determination of the rotationally invariant components of the stress tensor $\hat{\sigma}_{ik}$ in (12) (if any) in orthogonal transformation with (21) has the form

$$\forall\alpha : \hat{\sigma}'_{ik} \equiv (\underline{\underline{q}}^{\mathrm{T}}\cdot\underline{\underline{\hat{\sigma}}}\cdot\underline{\underline{q}})_{ik} = \hat{\sigma}_{ik}\,, \quad \hat{\sigma}^{\mathrm{T}\prime}_{ik} \equiv (\underline{\underline{q}}^{\mathrm{T}}\cdot\underline{\underline{\hat{\sigma}}}^{\mathrm{T}}\cdot\underline{\underline{q}})_{ik} = \hat{\sigma}^{\mathrm{T}}_{ik}\,. \tag{23}$$

Employing (22), we obtain that, with account for (7), the rotationally invariant components are determined from the conditions

$$\hat{\sigma}'_{11} \equiv \hat{\sigma}_{11}\,, \quad \hat{\sigma}'_{12} \equiv \hat{\sigma}_{12}\cos\alpha + \hat{\sigma}_{13}\sin\alpha = \hat{\sigma}_{12}\,, \quad \hat{\sigma}'_{13} \equiv -\,\hat{\sigma}_{12}\sin\alpha + \hat{\sigma}_{13}\cos\alpha = \hat{\sigma}_{13}\,. \tag{24}$$

The same relations hold for $\hat{\sigma}_{k1}$. The solution of the last two interrelated equations in (24) which are true for any α has the form $\hat{\sigma}_{12} = \hat{\sigma}_{21} = \hat{\sigma}_{13} = \hat{\sigma}_{31} = 0$. If the right-hand sides in (24) are replaced by $\hat{\sigma}_{ik}(1+O(\delta))$ and $\sigma^{T}_{ik}(1+O(\delta))$, where δ is a positive small parameter, it is easy to show that this case describes "nearly" rotationally invariant modes of shear stresses; these modes are responsible for the occurrence of semisoft behavior.

All the results obtained in this section can be formulated in the form of the following statement.

Theorem. *The shear stresses* $\hat{\sigma}_{1k}$ and $\hat{\sigma}_{k1}$ (k = 2 and 3) *in the constitutive equations (12) are rotationally (or nearly rotationally) invariant if and only if the modes* $\{1, k\}$ *are soft (semisoft); the set of soft (semisoft) shear modes has the power of a continuum.*

It is clear that for the free energy (4) rotational invariance occurs if and only if the condition of marginal stability (17) (or the condition of nearly marginal stability (18b)) is fulfilled. As is seen from (22) and (24), the rotationally (nearly rotationally) invariant mode of longitudinal stretching $\{11-22\}$ is not necessarily soft (semisoft). It is such if it is marginally (nearly marginally) stable. We note that the theorem of rotational invariance proved above is close to the principle of rotational invariance postulated by Olmsted [10].

4. Reduced Equations for Description of Soft Modes. If the shear modes $\{1, k\}$ are soft, the general solution of the problem for the constitutive equations (6) is complicated by the fact that the shear deformations $\hat{e}_{1k}$ in the soft modes are not uniquely determined. However, another important feature of soft shear modes exists, which makes solution of this problem more simple than that for the general stable case. The constitutive equations (12b) show that when the shear modes $\{1, k\}$ are soft, the antisymmetric components of the stress tensor in the coordinate system $\{\underline{\hat{x}}\}$ vanish since $\hat{\sigma}^{a}_{1k} = \hat{\sigma}^{a}_{k1} = 0$. This means that in the general case we have $\underline{\underline{\sigma}}^{a} = 0$ for weakly elastic nematic solid bodies with soft shear modes, i.e., *if the modes* $\{1, k\}$ *are soft, the stress tensor is symmetric.*

Employing the condition $\underline{\underline{\sigma}}^{a} = 0$ in (6b), we obtain

$$\underline{\underline{\omega}} = (G_3/G_4)\,(\underline{\underline{e}}\cdot\underline{n}\,\underline{n} - \underline{n}\,\underline{n}\cdot\underline{\underline{e}})\,. \tag{25}$$

This relation has been established in [9] on other grounds. Substituting (25) into (4) and (6a), we obtain the following expressions for the reduced free energy f^{r} and the symmetric reduced stress tensor $\underline{\underline{\sigma}}^{\mathrm{r}}$:

$$f^{\mathrm{r}} = \frac{1}{2}\,G_0\,|\underline{\underline{e}}|^2 + G^{\mathrm{r}}_1\underline{n}\,\underline{n} : \underline{\underline{e}}^2 + G^{\mathrm{r}}_2\,(\underline{n}\,\underline{n} : \underline{\underline{e}})^2\,, \tag{26}$$

$$\underline{\underline{\sigma}}^{\mathrm{r}} = G_0\underline{\underline{e}} + G^{\mathrm{r}}_1\,(\underline{n}\,\underline{n}\cdot\underline{\underline{e}} + \underline{\underline{e}}\cdot\underline{n}\,\underline{n}) + 2G^{\mathrm{r}}_2\underline{n}\,\underline{n}(\underline{\underline{e}} : \underline{n}\,\underline{n}) \quad (= \partial f^{\mathrm{r}}/\partial\underline{\underline{e}}!)\,, \tag{27}$$

$$G^{\mathrm{r}}_1 = G_1 - G^2_3/G_4\,, \quad G^{\mathrm{r}}_2 = G_2 + G^2_3/G_4\,. \tag{28}$$

Additionally, employing (1) together with (25), we find the expression for the director in a deformed state in the form

$$\underline{n}_{\rm d} = \underline{n} - \underline{\underline{\omega}}^{\rm B} \cdot \underline{n} + (G_3 / G_4)\, [\underline{\underline{e}} \cdot \underline{n} - \underline{n}\, (\underline{n}\,\underline{n} : \underline{\underline{e}})] \, . \tag{29}$$

We note that such a reduction is also justified when the condition $\underline{\underline{\sigma}}^{\rm a} = 0$ is fulfilled only approximately, as in the case of semisoft shear modes. Here the stability condition for the free energy (26) must be re-established. If (16) is fulfilled, relations (26)–(28) are simplified and take the form

$$\frac{f^{\rm r}}{G_0} = \frac{1}{2} \, |\underline{\underline{e}}|^2 - \underline{n}\,\underline{n} : \underline{\underline{e}}^2 + \frac{1}{4} \, (1 + 2\beta) \, (\underline{n}\,\underline{n} : \underline{\underline{e}})^2 \, , \tag{30}$$

$$\frac{\underline{\underline{\sigma}}^{\rm r}}{G_0} = \underline{\underline{e}} - (\underline{n}\,\underline{n} \cdot \underline{\underline{e}} + \underline{\underline{e}} \cdot \underline{n}\,\underline{n}) + \frac{1}{2} \, (1 + 2\beta) \, \underline{n}\,\underline{n} (\underline{\underline{e}} : \underline{n}\,\underline{n}) \, , \tag{31}$$

$$\beta = \left(\frac{3}{2} \, G_0 + 2G_1 + 2G_2 \right) \Big/ G_0 \geq 0 \, . \tag{32}$$

According to (16) and (18a), the parameter β is positive if the mode of longitudinal stretching $\{11 - 22\}$ is stable. If this stretching mode is also soft, we have $\beta = 0$ and the function $f^{\rm r}$ in (30) is minimized. Thus, the presence of both the stretching and shear soft modes leads to a minimum of the free energy f in the parametric space $\{P\}$. In this case, the right-hand sides of (30) and (31) for reduced expressions for the free energy and the stress tensor contain no parameters at all. This substantially simplifies the general analysis of deformations.

5. Weak Warner Potential. The general expression for this elastic potential has been derived by Warner et al. [15, 17] for nematic elastomers on the basis of a generalized Gauss kinetic theory of elasticity of rubbers; this theory allows for the presence of a liquid-crystalline order. Assuming that the parameters of molecular anisotropy $l_\|$ and $l_\perp$ remain constant under deformation, Olmsted [10] obtained an expression for the weak Warner potential, which (in our notation) has the form

$$\frac{f^{\rm W}}{G_0} = \frac{1}{2} \, |\underline{\underline{e}}|^2 + \frac{(\Delta l)^2}{4 l_\perp l_\|} \, [\underline{n}\,\underline{n} : \underline{\underline{e}}^2 - (\underline{n}\,\underline{n} \cdot \underline{\underline{e}})^2 - \underline{n}\,\underline{n} : \underline{\underline{\omega}}^2] - \frac{\Delta l^2}{2 l_\perp l_\|} \, \underline{n}\,\underline{n} : (\underline{\underline{e}} \cdot \underline{\underline{\omega}}) \, ,$$

$$(\Delta l)^2 = (l_\| - l_\perp)^2 \, , \quad \Delta l^2 = l_\|^2 - l_\perp^2 \, . \tag{33}$$

This expression represents a particular case of the free energy of de Gennes (4), where

$$G_1 = - G_2 = G_4 = G_0 \, \frac{(l_\| - l_\perp)^2}{l_\| l_\perp} \, , \quad G_3 = G_0 \, \frac{l_\|^2 - l_\perp^2}{l_\| l_\perp} \, . \tag{34}$$

Thus, the constitutive equations (6) for extra stresses are true in the case of the potential (33) with specification of the elastic moduli (34). It is seen that the parameters of (34) satisfy the condition of marginal stability (17) for the shear modes $\{1, k\}$ along with other constraints of thermodynamic stability in (13).

It follows that the *shear modes* $\{1, k\}$ *determined with the use of the potential (33) are always soft*, and the procedure of reduction to expressions (30) and (31) is fulfilled for (33) with a particular value of 3/2 for the parameter β. By virtue of this fact, the parameters of (34) do not describe marginal-stability constraint (16) for the stretching mode $\{11 - 22\}$. In such a description, it is not soft; a possible reason for this is that it is assumed that in the elastic potential (33), the parameters $l_\|$ and $l_\perp$ characterizing the anisotropy of the statistical properties of polymer chains are constant in the case of deformation.

6. Examples of Soft Elastic Deformations. Using Eqs. (30)–(32), we consider two simple cases of soft elastic nematic deformations.

6.1. Simple Shear. Let us employ the notation of Cartesian coordinate axes in simple shear: x_1 is arranged along the direction of displacement, x_2 is guided along the direction of the displacement gradient, and x_3 is oriented perpendicularly to them. In this case, the tensor of elastic deformations has only the following nonzero components: $e_{12} = e_{21} = \gamma/2$. Substituting them into (30) in the general case where $\underline{n}\,\underline{n}$ is a three-dimensional tensor, we obtain

$$2f^{\mathrm{r}}/(G\gamma^2) = n_3^2 + (1 + 2\beta)\, n_1^2 n_2^2 \quad (n_1^2 + n_2^2 + n_3^2 = 1)\ . \tag{35}$$

We have

$$\min f^{\mathrm{r}} = 0\ , \quad \text{when} \quad n_1 = 1 \quad (n_2 = n_3 = 0) \quad \text{or} \quad n_2 = 1 \quad (n_1 = n_3 = 0)\ ,$$

$$\max f^{\mathrm{r}} = \begin{cases} G_0\gamma^2/4\ , \quad n_3 = 1 \quad (n_1 = n_2 = 0)\ , \quad 0 \le \beta \le 1/2\ ; \\ G_0\gamma^2 \dfrac{1 + 6\beta}{8\,(1 + 2\beta)}\ , \quad n_1 = n_2 = \pm \dfrac{1}{\sqrt{(1 + 2\beta)}}\ , \quad \beta \ge 1/2\ . \end{cases} \tag{36}$$

It is seen that the zero free energy characteristic of the soft modes of nematic solid bodies is observed in simple shear when the initial director is oriented along the direction of shear x_1 or perpendicularly to it x_2. In orientation of the initial director along the x_3 axis and when $0 \le \beta \le 1/2$, free energy takes its maximum value equal to the corresponding value in an isotropic state. The value of the parameter $\beta = 0$ minimizes the free energy in simple shear.

The components of the reduced extra-stress tensor $\underline{\underline{\tilde{\sigma}}}^{\mathrm{r}} = 2\underline{\underline{\tilde{\sigma}}}^{\mathrm{r}}/(G_0\gamma)$ are determined as follows:

$$\tilde{\sigma}_{11}^{\mathrm{r}} = n_1 n_2\,[(1/2 + \beta)\, n_1^2 - 2]\ , \quad \tilde{\sigma}_{22}^{\mathrm{r}} = n_1 n_2\,[(1/2 + \beta)\, n_2^2 - 2]\ , \quad \tilde{\sigma}_{33}^{\mathrm{r}} = n_1 n_2\,(1/2 + \beta)\, n_3^2\ ,$$
$$\tilde{\sigma}_{12}^{\mathrm{r}} = n_3^2 + (1/2 + \beta)\, n_1^2 n_2^2\ , \quad \tilde{\sigma}_{23}^{\mathrm{r}} = n_1 n_3\,[(1/2 + \beta)\, n_2^2 - 1]\ , \quad \tilde{\sigma}_{13}^{\mathrm{r}} = n_2 n_3\,[(1/2 + \beta)\, n_1^2 - 1]\ . \tag{37}$$

It is seen that the zero extra-stress tensor characteristic of soft nematics is observed when the initial director is guided in parallel to the shear planes or perpendicularly to them. In orientation of the initial director perpendicularly to the $\{x_1x_2\}$ plane, it has only one component $\sigma_{12}^{\mathrm{r}} = G_0\gamma/2$ characteristic of the isotropic phase. In the general case where all n_i are more than 0, the components of the extra-stress tensor are positive, except for σ_{11}^{r} and σ_{22}^{r}. Because of this, the tensor of rotation of the entire body $\underline{\underline{\omega}}^{\mathrm{B}}$ has only two nonzero components: $\omega_{21}^{\mathrm{B}} = -\omega_{12}^{\mathrm{B}} = \gamma/2$. The components of the director $\underline{n}_{\mathrm{d}}$ in simple shear are determined, according to (29), in the form

$$n_{\mathrm{d}1} = n_1 + (\gamma/2)\, n_2\,[1 + (1 - 2n_1^2)\, G_3/G_4]\ , \quad n_{\mathrm{d}2} = n_2 + (\gamma/2)\, n_1\,[-1 + (1 - 2n_2^2)\, G_3/G_4]\ ,$$
$$n_{\mathrm{d}3} = n_3\,(1 - n_1 n_2 \gamma/G_3/G_4)\ . \tag{38}$$

These formulas characterize the position of the director in a deformed state $\underline{n}_{\mathrm{d}}$ for soft shear modes, when the initial director is guided along the shear x_1 or perpendicularly to it x_2.

6.2. Simple Tension. In this case, the tensor of elastic deformations has the form $\underline{\underline{e}} = \varepsilon \cdot \underline{\underline{\mathrm{diag}}}\,\{1, -1/2, -1/2\}$. It can be shown that simple tension exists for nematic solid bodies if and only if the director is guided along the tension axis, i.e., $\underline{n} = \{1, 0, 0\}$. Other orientations of the initial director in simple tension are accompanied by the appearance of shear stresses. Substituting these expressions into (30) and (31), we obtain

$$f^{\mathrm{r}} = G_0\varepsilon^2\beta/2\ , \quad \underline{\underline{\sigma}}^{\mathrm{r}} = G_0\varepsilon \cdot \underline{\underline{\mathrm{diag}}}\,\{\beta - 1/2, -1/2, -1/2\}\ . \tag{39}$$

Here $\underline{\underline{\sigma}}^{\mathrm{r}}$ is the reduced tensor of extra stresses. In uniaxial tension, the expression for elongation stress has the form

$$\sigma_{\mathrm{el}} \equiv \sigma_{11}^{\mathrm{r}} - \sigma_{22}^{\mathrm{r}} = G_0\varepsilon\beta\ . \tag{40}$$

In the case of the existence of soft shear/stretching modes where $\beta = 0$, the elongation stress for weakly elastic nematic solid bodies vanish together with the corresponding free energy.

CONCLUSIONS

This work has been motivated by the attempt of the authors to apply general formalism to description of the behavior of different anisotropic polymer systems (not only soft nematic elastomers) in equilibrium and nonequilibrium situations (see, for example, [25, 26]). Along with very soft nematic elastomers and gels, there are also semisoft and even hard nematic bodies. Furthermore, there are composites of liquid-like polymers filled with mutually attracting anisotropic (micro/nano-scale size) particles which exhibit nematic elastic properties characterized by relatively low stresses. The behavior of these nematic polymer systems with different degrees of rigidity cannot simply be described in terms of spontaneous breaking of isotropic symmetry [20].

In the work, the existence and description of soft, semisoft, and harder modes for weakly elastic nematic solid bodies have been studied on the basis of the de Gennes free energy [1] formulated on phenomenological grounds. The analysis has been substantially simplified on changing over to a special Cartesian coordinate system one axis of which is guided along the director. The following new results have been obtained:

1. The free energy (4) predicts that soft and semisoft modes exist if and only if the conditions of marginal (or nearly marginal) stability are fulfilled. Along with soft shear modes, the elastic potential (4) also predicts the existence of marginally stable soft and semisoft modes of longitudinal stretching.

2. If marginally stable nematic shear modes exist, the stress tensor is symmetric. In this case, the description of shear modes on the basis of the reduced expression f^{r} for free energy is simplified. The function f^{r} normalized by the isotropic elastic modulus contains only one dimensionless material parameter. It has been shown that this reduced consideration is always applicable to a weak version of the potential of Warner et al. [10, 15], which, however, does not predict the existence of the soft mode of longitudinal stretching. The presence of both, stretching and shear, soft modes minimizes the reduced free energy. In this case it contains no material parameters at all.

3. The theorem on rotational invariance that establishes the equivalence between the existence of soft shear modes and the rotational invariance of shear stress has been proved. It is close to the principle of rotational invariance postulated earlier by Olmsted [10].

4. Consideration has been given to examples of soft elastic deformations of solid bodies with internal stresses in simple shear and simple tension which exists only for the director guided along the tension axis. They demonstrate the large economy of the reduced free energy and of stresses as compared to the corresponding isotropic case.

Also, it should be noted that the elastic moduli G_k in (4) can variously depend on temperature. Therefore, the constraints (16) and (17) imposed on these material parameters by marginal stability (or nearly marginal stability) are able to generally exist only in certain temperature intervals.

NOTATION

$\underline{\underline{e}}$, deformation tensor; $\hat{e}_{ij}$, components of the deformation tensor in $\{\hat{\underline{x}}\}$; f, free energy; f^{r}, reduced free energy; $\hat{f}$, free energy in $\{\hat{\underline{x}}\}$; f^{W}, Warner potential; G_k, μ_k, and α_k, elastic moduli; $\{i, j\}$, nematic modes; $l_{\parallel}$ and $l_{\perp}$, parameters of molecular anisotropy; $\underline{n}$, initial director; $\underline{n}_{\mathrm{d}}$, director in a deformed state; p, isotropic pressure; Q, order parameter; Q_0, order parameter in an undeformed state; $\underline{\underline{q}}$, orthogonal matrix; $\underline{\underline{R}}$, orthogonal tensor of rotation of the director; tr $\underline{\underline{e}}$, trace of the deformation tensor; $\underline{u}$, displacement vector of a material point; $\{\hat{\underline{x}}\}$, special Cartesian coordinate system; $\nabla\underline{u}$, gradient of the displacement vector; β, scalar parameter; γ, shear; δ, parameter; $\underline{\underline{\delta}}$, unit tensor; δ_{ijk}, unit antisymmetric tensor; ε, tension; δ_{el}, elongation stress; $\hat{\sigma}_{\mathrm{el}}$, elongation stress in $\{\hat{\underline{x}}\}$; $\underline{\underline{\sigma}}$, extra-stress tensor; $\hat{\sigma}_{ij}$, components of the extra-stress tensor in $\{\hat{\underline{x}}\}$; $\underline{\underline{\sigma}}^{\mathrm{r}}$, reduced tensor of extra stresses; $\underline{\underline{\sigma}}^{\mathrm{s}}$ and $\underline{\underline{\sigma}}^{\mathrm{a}}$, symmetric and antisymmetric parts of the stress tensor; $\underline{\omega}^{\mathrm{I}}$, vector of internal rotation; $\underline{\underline{\omega}}$, relative-rotation tensor; $\hat{\omega}_{ij}$, components of the relative-rotation tensor in $\{\hat{\underline{x}}\}$; $\underline{\underline{\omega}}^{\mathrm{B}}$, tensor of rotation of the entire body; $\underline{\underline{\omega}}^{\mathrm{I}}$, internal-rotation tensor. Subscripts and superscripts: r, reduced; d, deformed; el, elongation; s, symmetric; a, antisymmetric; I, internal; B, body; T, transposition.

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