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Mesoscopic model for the viscosities of nematic liquid crystals

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Based on the definition of the mesoscopic concept by Blenk *et al.* [Physica A **174**, 119 (1991); J. Noneq. Therm. **16**, 67 (1991); Mol. Cryst. Liq. Cryst. **204**, 133 (1991)] an approach to calculate the Leslie viscosity coefficients for nematic liquid crystals is presented. The approach rests upon the mesoscopic stress tensor, whose structure is assumed similar to the macroscopic Leslie viscous stress. The proposed form is also the main dissipation part of the mesoscopic Navier-Stokes equation. On the basis of the correspondence between microscopic and mesoscopic scales a mean-field mesoscopic potential is introduced. It allows us to obtain the stress tensor angular velocity of the free rotating molecules with the help of the orientational Fokker-Planck equation. The macroscopic stress tensor is calculated as an average of the mesoscopic counterpart. Appropriate relations among mesoscopic viscosities have been found. The mesoscopic analysis results are shown to be consistent with the diffusional model of Kuzuu-Doi and Osipov-Terentjev with the exception of the shear viscosity α_4. In the nematic phase α_4 is shown to have two contributions: isotropic and nematic. There exists an indication that the influence of the isotropic part is dominant over the nematic part. The so-called microscopic stress tensor used in the microscopic theories is shown to be the mean-field potential-dependent representation of the mesoscopic stress tensor. In the limiting case of total alignment the Leslie coefficients are estimated for the diffusional and mesoscopic models. They are compared to the results of the affine transformation model of the perfectly ordered systems. This comparison shows disagreement concerning the rotational viscosity, whereas the coefficients characteristic for the symmetric part of the viscous stress tensor remain the same. The difference is caused by the hindered diffusion in the affine model case. [S1063-651X(99)11410-7]

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INTRODUCTION

The viscous stress tensor $\boldsymbol{\sigma}$ is a crucial part of the macroscopic Navier-Stokes equation that governs flow of the medium. In the case of liquid crystals, anisotropy of the system leads to numerous terms and viscosity coefficients in this tensor in order to describe flow properties. Recently there has been much interest in calculating nematic viscosities. A common approach uses statistical models [1–13] based on the Fokker-Planck (FP) equation approach introduced by Hess [14] and Doi [15]. These theories have revealed that the viscosity coefficients can be expressed as certain polynomials in local equilibrium orientational order parameters multiplied by a factor depending on the particle geometry and the rotational diffusion coefficient. This property has been intuitively taken for granted in some previous theoretical and experimental attempts to explain viscosity phenomena. By analogy to the Navier-Stokes equation, a mesoscopic counterpart of the stress tensor $\boldsymbol{\sigma}^{\text{mes}}$ is a matter of importance in the balance equation for the orientation-dependent mesoscopic momentum. A general form of this equation, along with the orientational balances for mass, spin, energy, and alignment tensors, have been derived in [16] in terms of the position $\mathbf{x}$, the microscopic director $\mathbf{a}$, and the time t variables. In this description the whole information about the order of the system is exclusively contained in the probabilistic orientational distribution function (ODF). The fact that the order parameters appear explicitly in the expressions for the viscosity coefficients in the FP theories indicates that $\boldsymbol{\sigma}^{\text{mes}}$ contains, besides ODF, components of the orientational variable $\mathbf{a}$. A particular form of $\boldsymbol{\sigma}^{\text{mes}}$ not only would complete knowledge about orientational balances but also would allow us to perform viscosity analysis that might lead to wider understanding of the mechanism, which finally gives order dependence of the viscosities.

The purpose of the paper is to calculate the Leslie viscous coefficients from the proposed general form of the mesoscopic stress tensor $\boldsymbol{\sigma}^{\text{mes}}$. A theoretical paper with a similar purpose has been done in [17]. In this paper the authors have combined features of the partially aligned systems composed of the rigid ellipsoidal particles with the predictions from the affine transformation (AT) model [18]. The main idea of the AT model is to relate physical properties of a perfectly aligned anisotropic fluid to those of a linearly viscous isotropic fluid by the use of the affine variable transformation. As

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a result a stress tensor expressed in components of the orientational variable **a** has been obtained. This form has been applied in [17] for the case of the partially aligned systems. The paper provides a very good insight into the problem. However, the predictions about the rotational viscosity are not in accordance with the Ericksen-Leslie continuum theory [19–21]. A rotational viscosity tensor is predicted instead of the usual scalar rotational viscosity. Consequently, the Parodi relation cannot be fulfilled. This is an effect of the assumed hindered particle rotations.

The presented mesoscopic approach is consistent with the microscopic models. Moreover, it naturally includes the isotropic contribution to the shear viscosity α_4 *in the anisotropic phase.* Although a severe disagreement between theoretical results and the experimental data for α_4 has already been noticed [12], not much theoretical indication has existed so far about the role of the isotropic effect.

The paper is organized as follows. Section I provides the necessary phenomenological definitions. Section II introduces the mesoscopic concept of orientational balances, velocities, and stress tensor. In Sec. III a derivation of the macroscopic stress tensor based on the mesoscopic description is presented. In Sec. IV a derivation of the total alignment limit for the viscosity coefficients is given by the Kuzuu-Doí and Osipov-Terentjev (KD-OT) approaches and compared to the result of the original AT model. Special attention has been paid to the rotational coefficient γ_1. In Sec. V we give a summary of the mesoscopic-approach conclusions and results.

I. PHENOMENOLOGY

Ericksen-Leslie stress tensor. In the Ericksen-Leslie (EL) theory [19–21] a unit vector, or ''director'' **n**, is introduced to represent the macroscopic symmetry axis at each point in space. The stress tensor $\boldsymbol{\sigma}$ is assumed to depend on the velocity gradients $\nabla\mathbf{v}$, the director **n**, and a corotational time derivative of the director **N**. For an incompressible nematic liquid crystal, it reads

$$\boldsymbol{\sigma}=\alpha_1\mathbf{nn}(\mathbf{nn}:\boldsymbol{\Gamma})+\alpha_2\mathbf{nN}+\alpha_3\mathbf{Nn}+\alpha_4\boldsymbol{\Gamma}+\alpha_5\mathbf{n}\boldsymbol{\Gamma}\cdot\mathbf{n}+\alpha_6\boldsymbol{\Gamma}\cdot\mathbf{nn}, \tag{1}$$

where we have used

$$\boldsymbol{\Gamma}\equiv\tfrac{1}{2}[\nabla\mathbf{v}+(\nabla\mathbf{v})^T],$$

$$\boldsymbol{\Omega}\equiv\tfrac{1}{2}[\nabla\mathbf{v}-(\nabla\mathbf{v})^T],$$

$$\mathbf{N}\equiv\dot{\mathbf{n}}+\boldsymbol{\Omega}\cdot\mathbf{n}, \tag{2}$$

and $[\boldsymbol{\Omega}\cdot\mathbf{n}]_i=\Omega_{ij}n_j$. As usual, the isotropic terms have been incorporated into the pressure. The viscosity constants $\alpha_1,\ldots,\alpha_6$ are the Leslie viscosity coefficients and the whole equation (1) is known as the first constitutive Leslie equation.

The antisymmetric part of Eq. (1),

$$\boldsymbol{\epsilon}:\boldsymbol{\sigma}=\mathbf{n}\times[-\gamma_1\mathbf{N}-\gamma_2(\boldsymbol{\Gamma}\cdot\mathbf{n})], \tag{3}$$

($\boldsymbol{\epsilon}$ is the completely antisymmetric unit tensor) contains the so-called rotational viscosity coefficients γ_1 and γ_2 defined by $\gamma_1\equiv\alpha_3-\alpha_2$ and $\gamma_2\equiv\alpha_6-\alpha_5$. They determine the viscous torques acting on the molecule: γ_1 is characteristic of the torque associated with the angular velocity of the director and γ_2 gives the strength of the torque in the shear flow. Another important parameter commonly used in hydrodynamics is the tumbling parameter $\lambda\equiv-\gamma_2/\gamma_1$, which for $|\lambda|\leq1$ is related to the flow alignment angle.

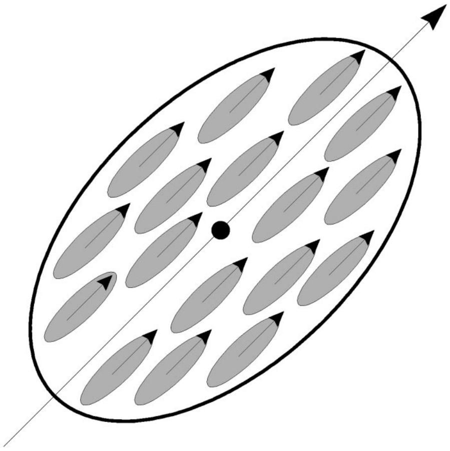

FIG. 1. A primitive view of the mesoscopic coarse grain. The orientation of the grain is assumed to agree with the particle orientation and the mesoscopic potential is assumed to agree with the mean-field potential acting on the individual molecule.

The EL theory can be extended by including the effect of external fields like magnetic, electric, or elastic deformations, in the form of the molecular field $\mathbf{h}_{\mathrm{mol}}$. In this case the energetically favorable state is obtained according to the rule

$$\mathbf{0}=\mathbf{n}\times(\mathbf{h}_{\mathrm{mol}}-\gamma_1\mathbf{N}-\gamma_2\boldsymbol{\Gamma}\cdot\mathbf{n}). \tag{4}$$

Due to Eq. (4) the director has to attain such an orientation that the effective torque, or the asymmetric part of the stress tensor, vanishes. This principle of angular momentum balance in nematics is known as the director equation or the second Leslie constitutive equation.

As pointed out in the Introduction, our goal is to show that the viscosities α_i, γ_i, and λ of nematic liquid crystals can be calculated on the basis of the mesoscopic orientational balances, thus to form a bridge between this type of description and the Fokker-Planck theories.

II. MESOSCOPIC CONCEPT

A. Orientational balances

In mesoscopic hydrodynamic description a liquid crystal is treated as an anisotropic medium requiring additional independent orientational variables in the domain of the field quantities as *the microscopic director* **a** and its *orientation change velocity* $\mathbf{w}(\mathbf{a},\mathbf{x},t)\equiv\partial\mathbf{a}/\partial t$, with the property $\mathbf{w}(\mathbf{a},\mathbf{x},t)\cdot\mathbf{a}=0$. Because in a mesoscopic grain all the molecules are assumed to be ordered due to the vector **a**, it is also possible to identify the microscopic director as the long principal axis of the molecule (see Fig. 1). Fields of physical quantities defined on the nematic space $(\cdot)\equiv(\mathbf{a},\mathbf{x},t)\in S^2\times R^3\times R^1$ are introduced in the mesoscopic concept. The second ingredient to a mesoscopic theory is the orientational distribution function $f(\cdot)$. As a statistical element $f(\cdot)d\mathbf{a}$ is regarded as the probability of finding a particle in the surface element $d\mathbf{a}$ around $\mathbf{a}$.

From the global balances of mass, momentum, angular momentum, and internal energy, it is possible to derive corresponding *local orientational balance equations.* For instance, the mass and momentum mesoscopic balances read

$$0=\frac{\partial}{\partial t}\rho(\cdot)+\boldsymbol{\nabla}_x\cdot[\rho(\cdot)\mathbf{v}(\cdot)]+\boldsymbol{\nabla}_n\cdot[\rho(\cdot)\mathbf{w}(\cdot)], \tag{5}$$

$$\begin{aligned}0=\frac{\partial}{\partial t}[\rho(\cdot)\mathbf{v}(\cdot)]&+\boldsymbol{\nabla}_x\cdot[\rho(\cdot)\mathbf{v}(\cdot)\mathbf{v}(\cdot)-\boldsymbol{\sigma}^T_{\mathrm{mes}}(\cdot)]\\&+\boldsymbol{\nabla}_n\cdot[\rho(\cdot)\mathbf{w}(\cdot)\mathbf{v}(\cdot)].\end{aligned} \tag{6}$$

Here, the orientational mass density is given by $\rho(\cdot)\equiv\rho(\mathbf{x},t)f(\cdot)$, where $f(\cdot)$ stands for the orientational distribution function and $\rho(\mathbf{x},t)$ is the macroscopic mass density at the point $\mathbf{x}$; $\mathbf{v}(\cdot)$ is the orientational material velocity (barycentric velocity of all molecules, whose orientation is given by the microscopic director $\mathbf{a}$ at position $\mathbf{x}$ at time t) and $\boldsymbol{\sigma}^T_{\mathrm{mes}}(\cdot)$ denotes the transposed mesoscopic (orientational) stress tensor. Orientational averages of these equations give back, by definition, the macroscopic mass balance and the Navier-Stokes equations, and also, consequently, the Leslie viscous stress tensor. However, with the exception of the Ehrentraut and Hess model [17], such a calculation or applications of this formalism to the description of liquid crystals properties has been missing. Note also that the mesoscopic concept can be applied to other nonequilibrium descriptions, which are based on the evolution of the probabilistic quantities like the dielectric relaxation processes [22,23].

A few words of explanation are needed about the applicability of the words *mesoscopic* and *microscopic*, for which an interchanged usage can be often met. The adjective *mesoscopic* in the standard definition refers to the coarse grains containing a large number of molecules. As compared to the macroscopic scale these grains are small enough to treat the system as a continuum in space. In a general sense the mesoscopic description includes more information than a macroscopic one, namely, the additional variable $\mathbf{a}$ in the domain of the mesoscopic fields. In the mesoscopic description neither notion of the molecular potential nor diffusivity have been used so far. On the other hand, the adjective *microscopic* is used in the models, which refer to an individual molecule's state or properties. In view of the above, the FP and AT models can be called *microscopic.*

B. Mesoscopic stress tensor in the affine transformation model

A structure of the mesoscopic stress tensor, a viscous stress tensor, which is defined on the mesoscopic variables, has appeared in consideration of the AT model [18]. Here we summarize the basic ideas of this model.

A volume-preserving transformation of a sphere into an ellipsoid of revolution of the axis ratio Q ($Q>1$ for rodlike particles, $Q<1$ for disclike particles) and the axis of symmetry $\mathbf{a}$,

$$\tilde{\mathbf{r}}=\mathbf{A}^{1/2}\cdot\mathbf{r}, \tag{7}$$

transforms a fluid of spheres into a fluid of anisotropic particles where the particles' axes are totally ordered. The transformation matrices are given by

$$\begin{aligned}\mathbf{A}&\equiv Q^{2/3}[\boldsymbol{\delta}+(Q^{-2}-1)\mathbf{aa}],\\ \mathbf{A}^{-1}&\equiv Q^{-2/3}[\boldsymbol{\delta}+(Q^{2}-1)\mathbf{aa}].\end{aligned} \tag{8}$$

It follows that the strain rates are related as

$$\tilde{\boldsymbol{\Gamma}}=\tfrac{1}{2}(\mathbf{A}^{-1/2}\cdot\boldsymbol{\nabla}\mathbf{v}\cdot\mathbf{A}^{1/2}+\mathbf{A}^{-1/2}\cdot(\boldsymbol{\nabla}\mathbf{v})^T\cdot\mathbf{A}^{1/2}). \tag{9}$$

With the usual assumption for the viscous stress tensor of an incompressible isotropic fluid $\tilde{\boldsymbol{\sigma}}=2\eta^{\mathrm{ref}}\tilde{\boldsymbol{\Gamma}}$, where η^{ref} is the shear viscosity of a reference fluid of spherical particles at the same density and temperature, the mesoscopic (viscous) stress tensor for the anisotropic fluid becomes

$$\begin{aligned}\boldsymbol{\sigma}^{\mathrm{ord}}&=\mathbf{A}^{-1/2}\cdot\tilde{\boldsymbol{\sigma}}\cdot\mathbf{A}^{1/2},\\ \boldsymbol{\sigma}^{\mathrm{ord}}&=\eta^{\mathrm{ref}}(\mathbf{A}^{-1}\cdot\boldsymbol{\nabla}\mathbf{v}\cdot\mathbf{A}+\boldsymbol{\nabla}\mathbf{v})\end{aligned} \tag{10}$$

(ord denotes perfectly ordered). Substituting Eq. (8) into Eq. (10) the following stress tensor in terms of the mesoscopic variables

$$\begin{aligned}\boldsymbol{\sigma}^{\mathrm{ord}}=\alpha_1^{\mathrm{ord}}\mathbf{aaaa}:\boldsymbol{\Gamma}&+\alpha_4^{\mathrm{ord}}\boldsymbol{\Gamma}+\alpha_5^{\mathrm{ord}}\mathbf{a}\boldsymbol{\Gamma}\cdot\mathbf{a}\\&+\alpha_6^{\mathrm{ord}}\boldsymbol{\Gamma}\cdot\mathbf{aa}+\alpha_2^{\mathrm{ord}}\mathbf{a}\boldsymbol{\Omega}\cdot\mathbf{a}+\alpha_3^{\mathrm{ord}}\boldsymbol{\Omega}\cdot\mathbf{aa}\end{aligned} \tag{11}$$

is obtained. While considering the case of the perfectly aligned ellipsoids, one can identify their symmetry axis $\mathbf{a}$ with the director $\mathbf{n}$ in the Ericksen-Leslie theory. The axis ratio Q is the only adjustable parameter in the AT model. The coefficients of the perfectly aligned fluid follow

$$\begin{gathered}\alpha_1^{\mathrm{ord}}=-\eta^{\mathrm{ref}}(Q-Q^{-1})^2,\quad \alpha_2^{\mathrm{ord}}=\eta^{\mathrm{ref}}(1-Q^2),\\ \alpha_3^{\mathrm{ord}}=\eta^{\mathrm{ref}}(Q^{-2}-1),\quad \alpha_4^{\mathrm{ord}}=2\eta^{\mathrm{ref}},\\ \alpha_5^{\mathrm{ord}}=-\alpha_2^{\mathrm{ord}},\quad \alpha_6^{\mathrm{ord}}=\alpha_3^{\mathrm{ord}},\\ \gamma_1^{\mathrm{ord}}=\alpha_3^{\mathrm{ord}}-\alpha_2^{\mathrm{ord}}=\eta^{\mathrm{ref}}(Q-Q^{-1})^2,\\ \gamma_2^{\mathrm{ord}}=\alpha_6^{\mathrm{ord}}-\alpha_5^{\mathrm{ord}}=\eta^{\mathrm{ref}}(Q^{-2}-Q^2),\\ \lambda=(1+Q^2)/(1-Q^2).\end{gathered} \tag{12}$$

In the above, in order to relate a part of the symmetric stress tensor to the rotational viscosity coefficient γ_2 the Parodi relation $\alpha_2^{\mathrm{ord}}+\alpha_3^{\mathrm{ord}}=\alpha_6^{\mathrm{ord}}-\alpha_5^{\mathrm{ord}}$ has been used.

C. Definition of the mesoscopic stress tensor

We follow the assumption from [17] that the dependence of the mesoscopic stress tensor on the mesoscopic variables becomes unchanged even if we allow the system to flow freely. However, the expression for the mesoscopic stress tensor should also contain information that the system is not perfectly aligned. This feature can be provided by the form of the orientational distribution function. Moreover, since the molecules can change their orientational position, $\boldsymbol{\sigma}_{\mathrm{mes}}$ should contain terms with the angular mesoscopic velocity $\mathbf{U}$. In the following we will use the ansatz for the mesoscopic stress tensor of the form

$$\boldsymbol{\sigma}_{\mathrm{mes}}(\cdot)=\alpha_1^{\mathrm{free}}\mathbf{aaaa}:\boldsymbol{\Gamma}f(\cdot)+\alpha_2^{\mathrm{free}}\mathbf{aU}f(\cdot)+\alpha_3^{\mathrm{free}}\mathbf{Ua}f(\cdot)+\alpha_4^{\mathrm{free}}\boldsymbol{\Gamma}f(\cdot)+\alpha_5^{\mathrm{free}}\mathbf{a}\boldsymbol{\Gamma}\cdot\mathbf{a}f(\cdot)+\alpha_6^{\mathrm{free}}\boldsymbol{\Gamma}\cdot\mathbf{aa}f(\cdot), \tag{13}$$

where

$$\mathbf{U}\equiv\dot{\mathbf{a}}+\boldsymbol{\Omega}\cdot\mathbf{a}. \tag{14}$$

We adopted here α_i^{free} values instead of the perfect order viscosities α_i^{ord} in order to account for the partial alignment dependence of the friction and the diffusion coefficients. The quantity $\boldsymbol{\sigma}^{\mathrm{mes}}(\mathbf{a},\mathbf{x},t)$ is the stress tensor of particles having the particular orientation $\mathbf{a}$ at point $\mathbf{x}$ in space. Note that ansatz (13) is such that it is in accordance with the Leslie macroscopic $\boldsymbol{\sigma}$ [Eq. (1)], which is a special assumption. It also fulfills the Parodi relation $\alpha_3^{\mathrm{free}}+\alpha_2^{\mathrm{free}}=\alpha_6^{\mathrm{free}}-\alpha_5^{\mathrm{free}}$.

III. MESOSCOPIC DERIVATION OF THE MACROSCOPIC STRESS TENSOR

The macroscopic stress tensor $\boldsymbol{\sigma}$ for the partially aligned fluid can be obtained by averaging the mesoscopic stress tensor $\boldsymbol{\sigma}^{\mathrm{mes}}(\cdot)$ [Eq. (13)] over all orientations. The main difficulty lies in the relationship between $\mathbf{U}$, the angular velocity of the microscopic director $\mathbf{a}$, and $\mathbf{N}$, the angular velocity of the macroscopic director $\mathbf{n}$. This problem can be resolved by considering links between the phenomenological and the mesoscopic theories.

Central to all kinetic theories is the diffusion equation for the time evolution of the orientation distribution function $f(\mathbf{a},t)$,

$$\frac{\partial f(\mathbf{a},t)}{\partial t}=D_r\mathbf{L}\cdot\left[\mathbf{L}f(\mathbf{a},t)+\frac{f(\mathbf{a},t)}{k_BT}\mathbf{L}V_{\mathrm{mf}}(\mathbf{a})\right]-\mathbf{L}\cdot[\boldsymbol{\Omega}^{\mathrm{Jef}}f(\mathbf{a},t)], \tag{15}$$

which describes the orientational Brownian motion of the particle in the mean-field potential $V_{\mathrm{mf}}(\mathbf{a})$. The long axis of the particle is given by the vector $\mathbf{a}$ and $\mathbf{L}=\mathbf{a}\times\boldsymbol{\nabla}_{\mathbf{a}}$ is the rotation operator, i.e., the covariant derivative on the S^2; $\boldsymbol{\Omega}^{\mathrm{Jef}}$ stands for the angular velocity gained by the particle under influence of the external velocity gradient field and D_r is the rotary diffusion coefficient. Because the system is assumed to be spatially homogenous, there is no position dependence in Eq. (15).

The mesoscopic counterpart of kinetic equation (15) originates from the balance law for mass density (5) [16]

$$0=\partial_t f(\cdot)+\boldsymbol{\nabla}_{\mathbf{x}}\cdot[\mathbf{v}(\cdot)f(\cdot)]+\boldsymbol{\nabla}_{\mathbf{a}}\cdot[\mathbf{w}(\cdot)f(\cdot)]+f(\cdot)[\partial_t+\mathbf{v}(\cdot)\cdot\boldsymbol{\nabla}_{\mathbf{x}}]\ln\rho(\mathbf{x},t). \tag{16}$$

Assuming that the system is uniform and incompressible, i.e., all gradients vanish except for $\boldsymbol{\nabla}\mathbf{v}$, which is not $\mathbf{x}$ dependent, Eq. (16) gives the equation [24]

$$\frac{\partial f(\mathbf{a},t)}{\partial t}+\mathbf{L}\cdot[\boldsymbol{\omega}_{\mathrm{mes}}f(\mathbf{a},t)]=0, \tag{17}$$

where the mesoscopic velocity $\boldsymbol{\omega}_{\mathrm{mes}}$ and the orientation change velocity $\mathbf{w}(\cdot)$ are related as

$$\boldsymbol{\omega}_{\mathrm{mes}}\equiv\mathbf{a}\times\mathbf{w}(\cdot). \tag{18}$$

Whether the two kinetic equations, Eqs. (15) and (17), can be compared is a subtle problem [25]. The first equation describes the state of an individual molecule influenced by the mean-field potential, whereas the second equation describes the orientation of the whole mesoscopic coarse grain. Here comes the most important assumption. To identify these two distribution functions as the same object we have to introduce implicitly the notion of the molecular potential field into the mesoscopic description by assuming that all molecules in the grain are perfectly ordered and reacting to the same mean-field potential (see Fig. 1). Comparison between the structures of Eqs. (15) and (17) gives then a particular form of the mesoscopic angular velocity $\boldsymbol{\omega}_{\mathrm{mes}}$,

$$\boldsymbol{\omega}_{\mathrm{mes}}=\boldsymbol{\Omega}^{\mathrm{Jef}}-D_r\mathbf{L}\left(\ln f+\frac{V_{\mathrm{mf}}}{k_BT}\right). \tag{19}$$

Equation (19) says that the instant effective mesoscopic angular velocity of the molecule is the velocity gained under influence of the macroscopic velocity gradient field diminished by the loss due to the diffusion processes of Brownian motion in the mean-field potential (so-called drift). For rigid ellipsoids of revolution an explicit form of $\boldsymbol{\Omega}^{\mathrm{Jef}}$ has been given by Jefferey [26],

$$\boldsymbol{\Omega}^{\mathrm{Jef}}=B\mathbf{a}\times(\boldsymbol{\Gamma}\cdot\mathbf{a})-\mathbf{a}\times(\boldsymbol{\Omega}\cdot\mathbf{a}), \tag{20}$$

where B is the shape form factor usually taken $B=(p^2-1)/(p^2+1)$, with p being the particle's axial length-to-width ratio.

Using expression (19) the angular velocity of the microscopic director $\mathbf{U}$ reads

$$\begin{aligned}\mathbf{U}&=\boldsymbol{\omega}_{\mathrm{mes}}\times\mathbf{a}+\boldsymbol{\Omega}\cdot\mathbf{a}\\&=(\boldsymbol{\delta}-\mathbf{aa})\cdot\left[B(\boldsymbol{\Gamma}\cdot\mathbf{a})-(\boldsymbol{\Omega}\cdot\mathbf{a})\right]\\&\quad-D_r\left[\mathbf{L}\left(\ln f+\frac{V_{\mathrm{mf}}}{k_BT}\right)\right]\times\mathbf{a}+\boldsymbol{\Omega}\cdot\mathbf{a}.\end{aligned} \tag{21}$$

In the above the first term on the right-hand side describes the hydrodynamic effect of the Jefferey-type due to the particle rotations caused by the velocity gradient field. The second term takes into account the diffusional reorientation effects. Although in the AT model internal free rotations are disallowed, there may still exist nonzero curl$\mathbf{v}$ and this effect is mirrored by the last part of Eq. (21). All these contributions are equally important.

The angular velocity of the form as in Eq. (21) has been applied to the evaluation of mesoscopic stress tensor (13) (see Appendix). Similarly to Eq. (21) in the stress tensor one can also distinguish three qualitative parts. The first part follows the structure, which is present in the original AT model.

The second part gives the contribution connected with the Jefferey angular motion and the third part takes into account the diffusional effects. All three parts contain symmetric velocity gradients, whereas the antisymmetric velocity gradients may occur only in the third diffusional term. It turns out, as compared to the KD-OT theory results, that evaluation of *only* the diffusional term can already give the whole stress tensor. From this argumentation it emerges that the affine-type stress and the Jefferey-type stress act as opposite effects, canceling each other.

A resultant expression for the stress tensor reads

$$\boldsymbol{\sigma}^{\mathrm{mes}}(\cdot)=-f(\cdot)D_r\left[\alpha_2^{\mathrm{free}}\mathbf{a}\frac{d}{d\mathbf{a}}\left(\ln f(\cdot)+\frac{V_{\mathrm{mf}}}{k_BT}\right)+\alpha_3^{\mathrm{free}}\frac{d}{d\mathbf{a}}\left(\ln f(\cdot)+\frac{V_{\mathrm{mf}}}{k_BT}\right)\mathbf{a}\right]+\alpha_4^{\mathrm{free}}\boldsymbol{\Gamma}f(\cdot) \tag{22}$$

and the following relations for the mesoscopic viscosities hold:

$$\begin{gathered}B\gamma_1^{\mathrm{free}}=-\gamma_2^{\mathrm{free}}\rightarrow\lambda^{\mathrm{free}}=B,\\ \alpha_1^{\mathrm{free}}=B(\alpha_2^{\mathrm{free}}+\alpha_3^{\mathrm{free}}),\\ B(\alpha_2^{\mathrm{free}}+\alpha_3^{\mathrm{free}})=-(\alpha_5^{\mathrm{free}}+\alpha_6^{\mathrm{free}}).\end{gathered} \tag{23}$$

Using Eq. (22) the symmetric and antisymmetric parts of the macroscopic stress tensor can be calculated as

$$\begin{gathered}\boldsymbol{\sigma}^{\mathrm{asym}}=\int f_0h\boldsymbol{\sigma}_{\mathrm{mic}}^{\mathrm{asym}}\mathrm{d}\mathbf{a},\\ \boldsymbol{\sigma}^{\mathrm{sym}}=\alpha_4^{\mathrm{free}}\boldsymbol{\Gamma}+\int f_0h\boldsymbol{\sigma}_{\mathrm{mic}}^{\mathrm{sym}}\mathrm{d}\mathbf{a},\end{gathered} \tag{24}$$

where

$$\boldsymbol{\sigma}_{\mathrm{mic}}^{\mathrm{asym}}=\frac{1}{k_BT}D_r\gamma_1^{\mathrm{free}}\frac{1}{2}\left(\mathbf{a}\frac{dV_{\mathrm{mf}}}{d\mathbf{a}}-\frac{dV_{\mathrm{mf}}}{d\mathbf{a}}\mathbf{a}\right), \tag{25}$$

and

$$\boldsymbol{\sigma}_{\mathrm{mic}}^{\mathrm{sym}}=\frac{1}{k_BT}D_r\gamma_1^{\mathrm{free}}B\left[3k_BT(\mathbf{aa}-\boldsymbol{\delta})+\frac{1}{2}\left(\mathbf{a}\frac{dV_{\mathrm{mf}}}{d\mathbf{a}}+\frac{dV_{\mathrm{mf}}}{d\mathbf{a}}\mathbf{a}\right)\right]. \tag{26}$$

In the above, h is the perturbation of the distribution function $f=f_0(1+h)$ linear in the velocity gradients and the equilibrium ODF is assumed as $f_0=\exp(-V_{\mathrm{mf}}/k_BT)$. In Eq. (26) we have also used the relation $-(\alpha_2^{\mathrm{free}}+\alpha_3^{\mathrm{free}})=\gamma_1^{\mathrm{free}}B$, which comes from the Parodi relation imposed on conditions (23). Also, since Eq. (25) relates to the molecular torque, which contains only the terms with the mean field potentials, the property

$$D_r\gamma_1^{\mathrm{free}}=k_BT \tag{27}$$

is expected to hold.

Equations (25) and (26) with Eq. (27) give the so-called microscopic stress tensor [27]—a stress tensor expressed in terms of the molecular mean-field potential, which originally has been introduced by Doi [15] through the considerations on the change of the free-energy caused by the external velocity field. It is not completely obvious on what grounds the results based on the free energy considerations coincide with the FP equation model. However, concluding from the calculation details it can be stated that the standard Brownian diffusion term relates to the change in the orientational entropy, whereas the mean potential drift relates to the change in the interaction term of the free energy.

Summing up the above considerations one can also arrive at another conclusive observation. Since the starting and the final expression have the form of statistical averages, both averaged quantities are the same. Thus the object $f_0h\boldsymbol{\sigma}_{\mathrm{mic}}$, which contains the microscopic stress tensor, can be regarded as the mean-field representation of the mesoscopic stress tensor.

In order to obtain explicit expressions for the Leslie viscosities one can follow now the calculation of the Osipov-Terentjev approach [4,12]. The main point of this model is the form of the distribution function. Since the flow breaks the cylindrical symmetry of a nematic, it has been suggested, within the assumption of low-velocity gradients, that the perturbation h should consist of all the combinations (there are four of them) of the velocity gradient and the components of the director **n** and the azimuth vector **e** multiplied with appropriate probabilistic functions. With this assumption it is possible to solve kinetic equation (15) almost completely in an analytical way and, next, calculate the macroscopic viscous stress tensor. Since the KD and OT approaches have been proven to lead to the equivalent results [12] for the expressions for the viscosity coefficients, we prefer the easier Kuzuu-Doi-like formulation to the convoluted integrals of the Osipov-Terentjev-type. The results for the viscosity coefficients are

$$\begin{gathered}\alpha_1=\alpha_1^{\mathrm{free}}S_4,\\ \alpha_2=\alpha_2^{\mathrm{free}}(1+\mu^{-1})S_2,\\ \alpha_3=\alpha_3^{\mathrm{free}}(1-\mu^{-1})S_2,\\ \alpha_4=\alpha_4^{\mathrm{free}}+\gamma_1^{\mathrm{free}}B^2\tfrac{1}{35}(7-5S_2-2S_4),\\ \alpha_5=\alpha_5^{\mathrm{free}}\left[\frac{B}{7}(3S_2+4S_4)+S_2\right],\\ \alpha_6=\alpha_6^{\mathrm{free}}\left[\frac{B}{7}(3S_2+4S_4)-S_2\right],\\ \gamma_1=\gamma_1^{\mathrm{free}}\mu^{-1}S_2,\\ \gamma_2=\gamma_2^{\mathrm{free}}S_2,\\ \mu=S_2\Big/\left\langle f_0\rho_a\frac{\partial V_{\mathrm{mf}}}{\partial\theta}\right\rangle,\end{gathered} \tag{28}$$

where ρ_a is one of the four components of h determined by the differential equation

$$\frac{d^2\rho_a}{d\theta^2}+\left(\cot\theta+\frac{1}{k_BT}\frac{dV_{\mathrm{mf}}}{d\theta}\right)\frac{d\rho_a}{d\theta}-\frac{\rho_a}{\sin^2\theta}=\frac{1}{k_BT}\frac{dV_{\mathrm{mf}}}{d\theta}. \tag{29}$$

For more details, see [3,12]. In the above we have used conditions (23) to show the relation between α_i and α_i^{free}.

The presented analysis, which starts from the mesoscopic background, coincides with the way of the microscopic KD-OT theory, with the exception of α_4. The main difference is that the mesoscopic approach naturally includes the isotropic contribution α_4^{free} to the shear viscosity α_4. So far, the existence of this contribution has not attracted enough attention. However, the importance is significant. There exists an indication that the isotropic α_4^{free} might be about ten times larger than the nematic part of α_4 [12]. Also, since α_4 enters all the viscosity values measured in the Miesowicz experiment, the lack of any molecular theory for α_4^{free} practically desists the KD-OT theory from successful application to analyze the experimental data for the Miesowicz coefficients [28]. To avoid this problem one should consider such differences between the Miesowicz coefficients in which the coefficient α_4 is eliminated.

IV. PERFECT ALIGNMENT LIMIT

Formulas (28) with respect to properties (23) and (27) present exactly the KD expressions (besides α_4^{free}). They should remain valid also in the special case of total alignment. Using the fact that all the order parameters are equal to unity in perfectly ordered systems the symmetric viscosities can be easily predicted,

$$\alpha_1^{\mathrm{ord}}=-\frac{k_BT}{D_r^{\mathrm{ord}}}B^2,$$

$$\alpha_2^{\mathrm{ord}}+\alpha_3^{\mathrm{ord}}=-\frac{k_BT}{D_r^{\mathrm{ord}}}B,$$

$$\alpha_5^{\mathrm{ord}}+\alpha_6^{\mathrm{ord}}=\frac{k_BT}{D_r^{\mathrm{ord}}}B^2,$$

$$\alpha_4^{\mathrm{ord}}=0. \tag{30}$$

By virtue of the Parodi relation the limit for the rotational coefficient γ_2 follows

$$\gamma_2^{\mathrm{ord}}=-\frac{k_BT}{D_r^{\mathrm{ord}}}B. \tag{31}$$

The second rotational coefficient γ_1 is more problematic. The common result of the OT and KD approaches is the integral

$$\gamma_1=\int f_0\rho_a\frac{dV_{\mathrm{mf}}}{d\theta}d\cos(\theta), \tag{32}$$

for which one cannot check the limit without solving the kinetic equation for the function ρ_a. Both, Eqs. (29) and (32), require knowledge of the particular mean-field potential. It has been noticed that the function ρ_a can also occur in the expression for $\alpha_2+\alpha_3$ in the OT formulation, which reads [12]

$$\alpha_2+\alpha_3=B\int f_0\rho_a\left(3k_BT\sin(2\theta)+\frac{dV_{\mathrm{mf}}}{d\theta}\cos(2\theta)\right)d\cos(\theta). \tag{33}$$

Using Eq. (30) the perfect-order limit of the integral on the right-hand side of Eq. (33) can be estimated as $(-k_BT/D_r)S_2$. This result imposes the property

$$\rho_a[\cos(\theta)=1]\frac{\partial V_{\mathrm{mf}}}{\partial\theta}[\cos(\theta)=1]=1, \tag{34}$$

where the perfect alignment equilibrium distribution function f_0 has been taken in the delta-function form $\delta(\cos(\theta)-1)$. Applying Eq. (34) to Eq. (32) the total alignment limit of the integral for γ_1 is obtained regardless the mean-field potential considerations,

$$\gamma_1^{\mathrm{ord}}=\frac{k_BT}{D_r^{\mathrm{ord}}}. \tag{35}$$

The relevant tumbling parameter reads

$$\lambda^{\mathrm{ord}}=B. \tag{36}$$

It can be useful to compare the obtained results, Eqs. (30), (31), (35), and (36), to the viscosity coefficients predicted by AT model (12). Introducing the formula for the rotational diffusion coefficient D_r,

$$D_r^{\mathrm{ord}}=\frac{k_BTQ^2}{\eta^{\mathrm{ref}}(Q^2+1)^2}, \tag{37}$$

one obtains the symmetric viscosities take identical forms in the affine, mesoscopic, or KD-OT theories, as already noticed in [9]. As far as the rotational coefficient γ_1 and the tumbling parameter $\lambda\equiv-\gamma_2/\gamma_1$ are concerned, the KD-OT model and the AT model lead to different predictions. The most illustrative is the result for the tumbling parameter, which in the KD-OT model is $\lambda=B$, whereas in the AT model, predicts $\lambda=B^{-1}$. Due to this disagreement the AT model cannot be applied to the description of the asymmetric viscosity in the systems where the reorientational processes are expected to be governed by the diffusion processes. This conclusion does not concern symmetric viscosity. The consistency between the results for the symmetric part of the stress tensor in the AT model and the perfect alignment limit of the KD-OT theory may be also the source of the information about the nature of the isotropic contribution $\alpha_4^{\rm free}$. Since the viscosity of the reference isotropic fluid $\eta^{\rm ref}$ by definition should remain indifferent to the strength of order of the anisotropic counterpart system, the AT model value $\alpha_4^{\rm ord}=2\eta^{\rm ref}$ can be considered as a general form of $\alpha_4^{\rm free}$ appearing in Eq. (28). This suggestion can be tested by the computer simulations.

V. DISCUSSION AND SUMMARY OF RESULTS

The idea of the aligned hard-rod system as simplification of freely rotating rods is quite common. It has led to a number of interesting predictions like stable transition from nematic to smectic *A* phase [29–31], depletion-driven nematic-nematic demixing transition [32], stable nematic columnar phase transition in binary mixtures of long and short rods [33], or S_2 dependence of the anisotropy of the diffusion constant [34]. Following this trend we have also used the conclusion of the AT model concerning the mesoscopic stress tensor [18,17], which is indispensable in the orientational balance equations for the analysis of the viscosity in the partially oriented systems with free particle rotations (Sec. III). The form of the stress tensor predicted by the AT model is completed with the terms responsible for the internal free rotations of the particles. The orientation distribution function that weights the AT-like expression is assumed to account for the strength of order of the system [Eq. (13)]. Moreover, for the mesoscopic viscosities we have adopted $\alpha_i^{\rm free}$ values instead of the perfect order viscosities $\alpha_i^{\rm ord}$ (as used in the original and modified AT approaches) in order to account for the order degree of the friction and diffusion coefficients in the case of partial alignment. As for the mesoscopic velocity we have used the deviation of the diffusional rotation velocity from the average angular velocity with which the particles rotate under influence of the external velocity gradient field. An expression for this velocity can be obtained from the FP equation [Eq. (19)]. In order to obtain the macroscopic stress tensor an orientational average of $\boldsymbol{\sigma}^{\rm mes}$ has been taken. This average can be transformed into another expression, also of a form of the statistical average, which contains the so-called microscopic stress tensor—a stress tensor expressed in terms of the molecular mean-field potential. These two averages are equivalent and may provide an interpretation of the microscopic stress tensor as a mean-field representation of the mesoscopic stress tensor. Calculation of the macroscopic stress involves three qualitative effects (Appendix). The first effect includes the stresses as considered in the standard AT model. The second effect represents the stresses due to the diffusion process and the third effect corresponds to the reaction of the particles to the velocity gradient field. The first and the latter contributions act in opposite ways. They cancel themselves leaving the diffusion effect mainly responsible for the viscosity. This calculation allows us also to obtain the particular values of the mesoscopic viscosities $\alpha_i^{\rm free}$, Eqs. (23) and (27). However, it has been observed that the symmetric contribution to the stress tensor obtained from the diffusional mean-field model coincides with the results of the AT models. This fact has led to the incorrect conclusion that the AT model, which does not take into account the possible reorientation of particles, holds in general.

Explicit Leslie viscosities can be calculated by the use of the KD-OT techniques [12]. The conclusions of the mesoscopic and the FP origin microscopic approaches are consistent with the exception of the shear viscosity α_4. More attention should be paid to this fact. In the mesoscopic approach it is clearly seen that the isotropic contribution to α_4, even in the nematic phase, is relevant. From the preliminary assessment [12] it might be ten times larger than the theoretically obtained nematic contribution. Because of this fact certain restrictions should be imposed on the comparison between the theories and the experimental data. For instance, in the Miesowicz experiment where all the measured viscosities contain α_4, one has to consider such combinations of the data coefficients that do not include α_4 in order to be able to apply the theoretical models for the data description. Alternatively, the need for separate measurements of the individual Leslie coefficients appears.

On the basis of viscosity expressions (28) we have calculated their total alignment limits and concluded about the anisotropy shape form factors associated with the particular viscosities in Sec. IV. Special attention has been paid to γ_1. It turns out that the comparison for the symmetric viscosities can be resolved in a consistent way with respect to an appropriate perfect order limit for diffusion coefficient (37). As far as the rotational properties are concerned disagreement between the AT model and the KD-OT has been pointed out. The presented analysis in Secs. III and IV highlights the correspondence between the total alignment approaches and the free particle rotations' models. So far, this relationship has remained unknown leaving the impression that the mentioned theories are contradictory.

To sum up, we have presented a mesoscopic approach to the viscosity theory of nematic liquid crystals, which is consistent with the microscopic descriptions in [3,12]. Our considerations show the necessity of further research on the nature of the rotational diffusion coefficients and the isotropic viscosity $\alpha_4^{\rm free}$ in the nematic phase. We hope that our results will help in future theoretical investigations of these properties.

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APPENDIX

Using the expression for the angular velocity of the microscopic director

$$\mathbf{U}=B(\boldsymbol{\Gamma}\cdot\mathbf{a})-(\boldsymbol{\Omega}\cdot\mathbf{a})-\mathbf{a}B(\boldsymbol{\Gamma}:\mathbf{aa})$$
$$-D_r\left[\mathbf{L}\left(\ln f+\frac{V_{\rm mf}}{k_BT}\right)\right]\times\mathbf{a}+\boldsymbol{\Omega}\cdot\mathbf{a}, \qquad (A1)$$

the mesoscopic stress tensor effectively will read

$$\begin{aligned}\boldsymbol{\sigma}_{\mathrm{mes}}(\cdot)/f(\cdot)&=\alpha_1^{\mathrm{free}}\mathbf{aa\Gamma}:\mathbf{aa}+\alpha_2^{\mathrm{free}}\mathbf{a}\left\{B\boldsymbol{\Gamma}\cdot\mathbf{a}-\mathbf{a}B\boldsymbol{\Gamma}:\mathbf{aa}-D_r\left[\mathbf{L}\left(\ln f+\frac{V_{\mathrm{mf}}}{k_BT}\right)\right]\times\mathbf{a}\right\}\\&\quad+\alpha_3^{\mathrm{free}}\left\{B\boldsymbol{\Gamma}\cdot\mathbf{a}-\mathbf{a}B\boldsymbol{\Gamma}:\mathbf{aa}-D_r\left[\mathbf{L}\left(\ln f+\frac{V_{\mathrm{mf}}}{k_BT}\right)\right]\times\mathbf{a}\right\}\mathbf{a}+\alpha_4^{\mathrm{free}}\boldsymbol{\Gamma}+\alpha_5^{\mathrm{free}}\mathbf{a}\boldsymbol{\Gamma}\cdot\mathbf{a}+\alpha_6^{\mathrm{free}}\boldsymbol{\Gamma}\cdot\mathbf{aa}\\&=\mathbf{aa\Gamma}:\mathbf{aa}(\alpha_1^{\mathrm{free}}-B\alpha_2^{\mathrm{free}}-B\alpha_3^{\mathrm{free}})+\alpha_4^{\mathrm{free}}\boldsymbol{\Gamma}+\mathbf{a}(\boldsymbol{\Gamma}\cdot\mathbf{a})(B\alpha_2^{\mathrm{free}}+\alpha_5^{\mathrm{free}})+(\boldsymbol{\Gamma}\cdot\mathbf{a})\mathbf{a}(B\alpha_3^{\mathrm{free}}+\alpha_6^{\mathrm{free}})\\&\quad+\alpha_2^{\mathrm{free}}D_r\mathbf{a}\left\{\left[\mathbf{a}\times\mathbf{L}\left(\ln f+\frac{V_{\mathrm{mf}}}{k_BT}\right)\right]\right\}+\alpha_3^{\mathrm{free}}D_r\left\{\left[\mathbf{a}\times\mathbf{L}\left(\ln f+\frac{V_{\mathrm{mf}}}{k_BT}\right)\right]\right\}\mathbf{a}.\end{aligned}\tag{A2}$$

In the above expression the antisymmetric velocity gradient tensor may appear only in the diffusional term. We will evaluate this term in the first order. We will be using the representation of the orientation variable **a** and its derivative $d/d\mathbf{a}$ as

$$\mathbf{a}=\mathbf{n}\cos\theta+\mathbf{e}\sin\theta,$$

$$\frac{d}{d\mathbf{a}}=(\mathbf{e}\cos\theta-\mathbf{n}\sin\theta)\frac{d}{d\theta}+\frac{\mathbf{n}\times\mathbf{e}}{\sin\theta}\frac{d}{d\varphi},\tag{A3}$$

where **e** is the azimuthal unit vector perpendicular to the director **n**; $\mathbf{a}\times\mathbf{L}=-d/d\mathbf{a}$; $da_j/da_i=\delta_{ij}-a_ia_j$ and $da_i/da_i=2$. The reference frame is chosen in a way that the components of the needed unit vectors read $e_x=\cos\varphi$, $e_y=\sin\varphi$, $e_z=0$, $n_x=n_y$, and $n_z=1$. A nontrivial formula for the integration by parts follows

$$\int d\mathbf{a}G\frac{dF}{da_i}=-\int d\mathbf{a}F\frac{dG}{da_i}+2\int d\mathbf{a}GFa_i,\tag{A4}$$

where $d\mathbf{a}=d\varphi d\cos\theta$. The diffusional part of the macroscopic stress tensor $\mathbf{I}_{\mathrm{diff}}$ reads [see Eq. (A2)]

$$\begin{aligned}\mathbf{I}_{\mathrm{diff}}=-D_r\int f(\cdot)\left[\alpha_2^{\mathrm{free}}\mathbf{a}\frac{d}{d\mathbf{a}}\left(\ln f+\frac{V_{\mathrm{mf}}}{k_BT}\right)\right.\\\left.+\alpha_3^{\mathrm{free}}\frac{d}{d\mathbf{a}}\left(\ln f+\frac{V_{\mathrm{mf}}}{k_BT}\right)\mathbf{a}\right]d\mathbf{a}.\end{aligned}\tag{A5}$$

Keeping only relevant terms linear in the velocity gradients like $f=f_0(1+h)$ and

$$\ln f=\ln f_0+\ln(1+h)=-\frac{V_{\mathrm{mf}}}{k_BT}+h,\tag{A6}$$

expression (A5) will look like

$$\mathbf{I}_{\mathrm{diff}}=-D_r\int d\mathbf{a}f_0\left[\alpha_2^{\mathrm{free}}\mathbf{a}\frac{dh}{d\mathbf{a}}+\alpha_3^{\mathrm{free}}\frac{dh}{d\mathbf{a}}\mathbf{a}\right].\tag{A7}$$

By the use of Eq. (A4) $\mathbf{I}_{\mathrm{diff}}$ can be evaluated as follows:

$$\begin{aligned}\mathbf{I}_{\mathrm{diff}}D_r^{-1}&=\int d\mathbf{a}h\left[\alpha_2^{\mathrm{free}}\frac{d(f_0a_i)}{da_j}+\alpha_3^{\mathrm{free}}\frac{d(f_0a_j)}{da_i}\right]\\&\quad-2\int d\mathbf{a}f_0ha_ia_j(\alpha_2^{\mathrm{free}}+\alpha_3^{\mathrm{free}})\\&=\int d\mathbf{a}h\left[\alpha_2^{\mathrm{free}}a_i\frac{df_0}{da_j}+\alpha_3^{\mathrm{free}}a_j\frac{df_0}{da_i}\right]\\&\quad+\int d\mathbf{a}f_0h\left[\alpha_2^{\mathrm{free}}\frac{da_i}{da_j}+\alpha_3^{\mathrm{free}}\frac{da_j}{da_i}\right]\\&\quad-2\int d\mathbf{a}f_0ha_ia_j(\alpha_2^{\mathrm{free}}+\alpha_3^{\mathrm{free}})\\&=-\frac{1}{k_BT}\int d\mathbf{a}hf_0\left[\alpha_2^{\mathrm{free}}a_i\frac{dV_{\mathrm{mf}}}{da_j}+\alpha_3^{\mathrm{free}}a_j\frac{dV_{\mathrm{mf}}}{da_i}\right]\\&\quad+\int d\mathbf{a}f_0h(\alpha_2^{\mathrm{free}}+\alpha_3^{\mathrm{free}})(\delta_{ij}-a_ia_j)\\&\quad-2\int d\mathbf{a}f_0ha_ia_j(\alpha_2^{\mathrm{free}}+\alpha_3^{\mathrm{free}}).\end{aligned}\tag{A8}$$

Splitting into the symmetric and antisymmetric parts gives

$$\begin{aligned}\mathbf{I}_{\mathrm{diff}}^{\mathrm{sym}}&=-\frac{D_r}{k_BT}(\alpha_2^{\mathrm{free}}+\alpha_3^{\mathrm{free}})\int d\mathbf{a}hf_0\left[k_BT(3a_ia_j-\delta_{ij})\right.\\&\quad\left.+\frac{1}{2}\left(a_i\frac{dV_{\mathrm{mf}}}{da_j}+a_j\frac{dV_{\mathrm{mf}}}{da_i}\right)\right]\\&=\int d\mathbf{a}\sigma_{ij}^{\mathrm{micr,sym}}hf_0,\end{aligned}\tag{A9}$$

$$\begin{aligned}\mathbf{I}_{\mathrm{diff}}^{\mathrm{asym}}&=-\frac{D_r}{k_BT}(\alpha_3^{\mathrm{free}}-\alpha_2^{\mathrm{free}})\int d\mathbf{a}hf_0\frac{1}{2}\left[a_i\frac{dV_{\mathrm{mf}}}{da_j}-a_j\frac{dV_{\mathrm{mf}}}{da_i}\right]\\&=\int d\mathbf{a}\sigma_{ij}^{\mathrm{micr,asym}}hf_0.\end{aligned}\tag{A10}$$

Formulas (A9) and (A10) agree with the stress tensor definition used in the KD-OT theory. This fact indicates that the AT model contribution to the stress is balanced by the Jeferey effect in expression (A2) and the relations

$$\begin{aligned}B\gamma_1^{\mathrm{free}}&=-\gamma_2^{\mathrm{free}},\\\alpha_1^{\mathrm{free}}&=B(\alpha_2^{\mathrm{free}}+\alpha_3^{\mathrm{free}}),\\B(\alpha_2^{\mathrm{free}}+\alpha_3^{\mathrm{free}})&=-(\alpha_5^{\mathrm{free}}+\alpha_6^{\mathrm{free}}),\end{aligned}\tag{A11}$$

must hold. In this case both different models are consistent.

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