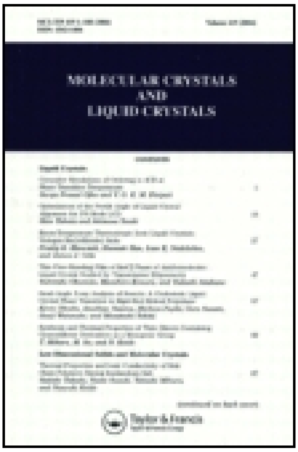

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Orientation-Balances for Liquid Crystals and Their Representation by Alignment Tensors

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Orientation-Balances for Liquid Crystals and Their Representation by Alignment Tensors

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1 INTRODUCTION

Up to now there are three different phenomenological concepts suitable to describe liquid crystals: The first one is the well known Ericksen-Leslie theory[4] whose balance equations are formulated by use of a *macroscopic director* for needle-shaped molecules with totally relaxed internal degrees of freedom. This macroscopic director is not well defined microscopically: It can not be identified with the orientation of a single molecule because the orientation of the molecules is statistically distributed. Therefore we need a distribution function for describing the orientation in the fluid, or we restrict ourselves to the case of total alignment. In that case the macroscopic director of the Ericksen-Leslie theory coincides with the common alignment of all molecules.

The second concept describing liquid crystals uses the alignment-tensor[7,13] which represents the first anisotropy moment of a multipole expansion of the orientation distribution function. We get an alignment tensor balance equation whose production term is caused by orientation-diffusion and orientation-relaxation.

The third concept describing liquid crystals is based on the idea that different orientations of molecules may be described as components of a mixture.[1,2] The index numbering the component is here the orientation, represented by two angles determining a point on the unit sphere. Because mixture theories are well developed[11,12] balance equations for liquid crystals can be written down very easily by use of this method. We get balance equations whose domain contains the *microscopic director* describing the individual orientation of one molecule.

The aim of this paper is to derive phenomenological balance equations for liquid crystals in alignment tensor formulation by use of a function defined on the 2-sphere describing the distribution of microscopic directors.

2 STATISTICAL FOUNDATION

The orientation of a single molecule of given position $\boldsymbol{x}$ and given velocity $\boldsymbol{v}$ is represented by the *microscopic director* $\boldsymbol{n}$ which is an element of the 2-sphere.

The change of the orientation is described by an orientational change velocity $\boldsymbol{u}$. Therefore we have a time-dependent distribution function f_t defined on the so called 10-dimensional *doubled phase space* $(\boldsymbol{x}, \boldsymbol{n}, \boldsymbol{v}, \boldsymbol{u}) \in \Omega$ which is spanned by the 6-dimensional one-particle phase space and by the 4-dimensional orientational 2-sphere state space. As usual the distribution function f_t represents the distribution density of the particles due to *position* $\boldsymbol{x}$ and *velocity* $\boldsymbol{v}$ of their centres of mass and due to their *orientation* $\boldsymbol{n}$ and their *orientational change velocity* $\boldsymbol{u}$ ($\boldsymbol{v} \equiv \dot{\boldsymbol{x}}(t)$ and $\boldsymbol{u} \equiv \dot{\boldsymbol{n}}(t)$) at a time t

$$f_t = f_t(\boldsymbol{x}, \boldsymbol{n}, \boldsymbol{v}, \boldsymbol{u}) \equiv f_t(\Box). \tag{1}$$

According to the nematic symmetry

$$f_t(\boldsymbol{x}, \boldsymbol{n}, \boldsymbol{v}, \boldsymbol{u}) = f_t(\boldsymbol{x}, -\boldsymbol{n}, \boldsymbol{v}, -\boldsymbol{u}) \quad \text{for all } (\boldsymbol{x}, \boldsymbol{n}, \boldsymbol{v}, \boldsymbol{u}) \in \Omega \tag{2}$$

is valid. We are able to use the usual gradients $\nabla_n \equiv \partial/\partial \boldsymbol{n}$ and $\nabla_u \equiv \partial/\partial \boldsymbol{u}$ and the well known integration theorem due to Stokes in IR^3 (either with respect to $\boldsymbol{n}$ or with respect to $\boldsymbol{u}$).[3] Balances are globally defined on the doubled phase space Ω and are treated in the next section.

3 GLOBAL BALANCE EQUATIONS ON Ω

In the doubled phase space each particle is represented by its 10 coordinates ($\boldsymbol{x}$, $\boldsymbol{u}$, $\boldsymbol{v}$, $\boldsymbol{u}$) at the time t. But in general there are more than one particle having at the same time the same coordinates according to the statistical approach using a distribution function. Since at later times particles of the same coordinates at earlier times may have different ones, particles can not be traced back uniquely. Hence the fundamental concept of a *body* in continuum physics[15] does not exist in a statistical approach using a distribution function.

Athough the concept of a body does not exist one is able to formulate global balance equations in the doubled phase space by choosing special domains of integration. These domains — called *modified bodies* — are characterized by the two following properties[3]:

1. The total convective flux of the balance quantity across the boundary of a modified body must vanish,
2. The total mass flux across the boundary of a modified body must vanish, too.

Hence the following general global balance can be formulated:

$$\frac{d}{dt}\int_{G_t} f_t(\Box)\phi(\Box)\,d^{10}\Omega = \int_{G_t}\left[f_t(\Box)\Psi_t(\Box) + \nabla_x\cdot\underline{\underline{J}}^{\mathrm{T}}_{\phi t}(\Box)\right]\,d^{10}\Omega \tag{3}$$

ϕ = balanced quantity $\qquad$ Ψ_t = production of ϕ

$\underline{\underline{J}}_{\phi t}$ = flux density belonging to ϕ

In this general balance the balances of mass, momentum, angular momentum and energy are included by a special choice of ϕ, Ψ_t, and $\underline{\underline{J}}_{\phi t}$. Formulated on Ω they can be reduced to the so-called orientation balance equations.

4 ORIENTATION BALANCE EQUATIONS

By definition orientation balance equations are formulated on the position part of Ω $(\boldsymbol{x}, \boldsymbol{n}) \in \Sigma \subset \Omega$. Therefore we get the orientation balance equations by integrating the balances defined on Ω over the velocity part of Ω: $(\boldsymbol{v}, \boldsymbol{u}) \in \Sigma' \subset \Omega$.

By this procedure we establish a series of averages on Σ' of the physical quantities which occur in the left hand side of the general global balance Equation (3).

$$\rho(\cdot)\phi(\cdot) := \int_{\Sigma'} \rho_t(\Box)\phi(\Box)\,d^5\Sigma'. \tag{4}$$

Here the abbreviation

$$(\cdot) \equiv (\boldsymbol{x}, \boldsymbol{n}, t) \tag{5}$$

is introduced for the set of variables belonging to Σ. For exploiting the total time derivative in the balance equation we need the commutation rule between the total time derivative and the integration. This rule is given by the *generalized Reynolds transport theorem*

Proposition 4.1

If $\Phi_t(\Box)$: $\Omega \times \mathrm{IR} \to \mathrm{IR}$ is continuously differentiable and $G_t \subset \Omega$, then

$$\frac{d}{dt}\int_{G_t}\Phi_t(\Box)\,d^{10}\Omega = \\ = \int_{G_t}\left\{\frac{\partial}{\partial t}\Phi_t(\Box) + \nabla_\Sigma\cdot\left(\boldsymbol{v}_M\Phi_t(\Box)\right) + \nabla_{\Sigma'}\cdot\left(\boldsymbol{u}_M\Phi_t(\Box)\right)\right\}d^{10}\Omega \tag{6}$$

is valid. ∇_Σ (resp. $\nabla_{\Sigma'}$) denotes the gradient of the appropriate variables $(\boldsymbol{x}, \boldsymbol{n}) \in \Sigma$ (resp. $(\boldsymbol{v}, \boldsymbol{u}) \in \Sigma'$) and $\boldsymbol{v}_M$ and $\boldsymbol{u}_M$ are the velocities of the time evolution of G_t projected on Σ or Σ', respectively.

Because we integrate the balance equations over all the velocities in Σ' we need:

Proposition 4.2

Presupposing suitable conditions[3,14] the following statements are valid

$$\int_{\Sigma'} \nabla_{\Sigma'} \cdot (\boldsymbol{u}_M f_t(\Box) X)\, d^5\Sigma' = 0 \qquad (X = \textit{mass, momentum, angular momentum, energy}) \tag{7}$$

$$\nabla_n \cdot (\boldsymbol{u}\Phi) = \boldsymbol{n} \cdot \nabla_n \times (\boldsymbol{n} \times \boldsymbol{u}\Phi) \ , \tag{8}$$

$$\int_{S^2} \nabla_n \cdot (\boldsymbol{u}\Phi)\, d^2 n = 0 \ . \tag{9}$$

By use of proposition 4.1 we get the following orientation balance equations defined on Σ

mass:

$$\frac{\partial}{\partial t}\rho(\cdot) + \nabla_x \cdot (\boldsymbol{v}(\cdot)\rho(\cdot)) + \nabla_n \cdot (\boldsymbol{u}(\cdot)\rho(\cdot)) = 0 \ , \tag{10}$$

momentum:

$$\begin{aligned} &\frac{\partial}{\partial t}\Big(\rho(\cdot)\boldsymbol{v}(\cdot)\Big) + \nabla_x \cdot \Big(\boldsymbol{v}(\cdot)\rho(\cdot)\boldsymbol{v}(\cdot) - \underline{\underline{\boldsymbol{T}}}^{\mathsf{T}}(\cdot)\Big) + \\ &+ \boldsymbol{n} \cdot \nabla_n \times \Big(\boldsymbol{\omega}(\cdot)\rho(\cdot)\boldsymbol{v}(\cdot) - \underline{\underline{\boldsymbol{U}}}^{\mathsf{T}}(\cdot)\Big) = \rho(\cdot)\boldsymbol{f}(\cdot) \ , \end{aligned} \tag{11}$$

spin:

$$\begin{aligned} &\Big(\frac{\partial}{\partial t} + \nabla_x \cdot \boldsymbol{v}(\cdot) + \nabla_n \cdot \boldsymbol{u}(\cdot)\Big)\rho(\cdot)(\theta\boldsymbol{\omega}(\cdot)) = \rho(\cdot)\boldsymbol{n} \times \boldsymbol{g}(\cdot) + \\ &\boldsymbol{n} \times \nabla_x \cdot \underline{\underline{\boldsymbol{\Pi}}}^{\mathsf{T}}(\cdot) + \boldsymbol{n} \cdot \nabla_n \times (\boldsymbol{n} \times \underline{\underline{\boldsymbol{\Xi}}}(\cdot))^{\mathsf{T}} + \underline{\epsilon_3} : \underline{\underline{\boldsymbol{T}}}(\cdot) \end{aligned} \tag{12}$$

internal energy:

$$\begin{aligned} &\frac{\partial}{\partial t}\Big(\rho(\cdot)\epsilon(\cdot)\Big) + \nabla_x \cdot \Big(\boldsymbol{q}(\cdot) + \rho(\cdot)\boldsymbol{v}(\cdot)\epsilon(\cdot)\Big) + \boldsymbol{n} \cdot \nabla_n \times \Big(\boldsymbol{Q}(\cdot) + \\ &\boldsymbol{\omega}(\cdot)\rho(\cdot)\epsilon(\cdot)\Big) = \rho(\cdot)r(\cdot) + (\nabla_x \boldsymbol{v}(\cdot)) : \underline{\underline{\boldsymbol{T}}}(\cdot) + (\nabla_x \boldsymbol{u}(\cdot)) : \underline{\underline{\boldsymbol{\Pi}}}(\cdot) \\ &-\boldsymbol{\omega}(\cdot) \cdot \underline{\epsilon_3} : \underline{\underline{\boldsymbol{T}}}(\cdot) + \boldsymbol{n} \cdot \Big((\nabla_n \cdot \underline{\epsilon_3}\boldsymbol{v}(\cdot)) : \underline{\underline{\boldsymbol{U}}}(\cdot) + (\nabla_n \cdot \underline{\epsilon_3}\boldsymbol{u}(\cdot)) : \underline{\underline{\boldsymbol{\Xi}}}(\cdot)\Big) \ . \end{aligned} \tag{13}$$

In these orientation balances the following basic fields per orientation occur

mass density:

$$\rho(\cdot) := \int_{\Sigma'} \rho_t(\Box)\, d^5\Sigma' \ , \tag{14}$$

velocity:

$$\rho(\cdot)\boldsymbol{v}(\cdot) := \int_{\Sigma'} \rho_t(\Box)\boldsymbol{v}\, d^5\Sigma' \ , \tag{15}$$

orientational change velocity and angular velocity:

$$\rho(\cdot)\boldsymbol{u}(\cdot) := \int_{\Sigma'} \rho_t(\square)\boldsymbol{u}\, d^5\Sigma'\ , \quad \boldsymbol{\omega}(\cdot) := \boldsymbol{n} \times \boldsymbol{u}(\cdot) \tag{16}$$

quadratic averages:

$$\rho(\cdot)(\boldsymbol{Y}\boldsymbol{v})(\cdot) := \int_{\Sigma'} \rho_t(\square)\boldsymbol{Y}\boldsymbol{v}\, d^5\Sigma' \quad \text{with } \boldsymbol{Y} = \boldsymbol{u}, \boldsymbol{v} \tag{17}$$

internal energy density:

$$\rho(\cdot)\left\{\frac{1}{2}\left[\boldsymbol{v}(\cdot)\right]^2 + \frac{1}{2}\theta\left[\boldsymbol{n} \times \boldsymbol{u}(\cdot)\right]^2 + \epsilon(\cdot)\right\} := \tag{18}$$

$$\int_{\Sigma'} \rho_t(\square)\left[\frac{1}{2}\boldsymbol{v}^2 + \frac{1}{2}\theta(\boldsymbol{n} \times \boldsymbol{u})^2 + \epsilon_t(\square)\right] d^5\Sigma'$$

force density per orientation:

$$\rho(\cdot)\boldsymbol{f}(\cdot) := \int_{\Sigma'} \rho_t(\square)\boldsymbol{k}_t(\square)\, d^5\Sigma'\ , \tag{19}$$

stress tensors:

$$\underline{\underline{\boldsymbol{T}}}(\cdot) \ := \ \int_{\Sigma'} \underline{\underline{\boldsymbol{P}}}_t(\square)\, d^5\Sigma' + \rho(\cdot)\Big(\boldsymbol{v}(\cdot)\boldsymbol{v}(\cdot) - (\boldsymbol{v}\boldsymbol{v})(\cdot)\Big)\ , \tag{20}$$

$$\underline{\underline{\boldsymbol{U}}}(\cdot) \ := \ \rho(\cdot)\Big(\boldsymbol{v}(\cdot)\boldsymbol{n} \times \boldsymbol{u}(\cdot) - (\boldsymbol{v}\boldsymbol{n} \times \boldsymbol{u})(\cdot)\Big)\ , \tag{21}$$

couple force:

$$\rho(\cdot)\boldsymbol{g}(\cdot) := \int_{\Sigma'} \rho_t(\square)\boldsymbol{g}_t(\square)\, d^5\Sigma'\ , \tag{22}$$

couple stress tensors:

$$\underline{\underline{\boldsymbol{\Pi}}}(\cdot) \ := \ \int_{\Sigma'} \underline{\underline{\boldsymbol{\pi}}}_t(\square)\, d^5\Sigma' + \theta\rho(\cdot)\Big(\boldsymbol{u}(\cdot)\boldsymbol{v}(\cdot) \ - \ (\boldsymbol{u}\boldsymbol{v})(\cdot)\Big), \tag{23}$$

$$\underline{\underline{\boldsymbol{\Xi}}}(\cdot) \ := \ \theta\rho(\cdot)\Big(\boldsymbol{u}(\cdot)\boldsymbol{n} \times \boldsymbol{u}(\cdot) \ - \ (\boldsymbol{u}\boldsymbol{n} \times \boldsymbol{u})(\cdot)\Big)\ , \tag{24}$$

heat fluxes:

$$\begin{aligned} \boldsymbol{q}(\cdot) \ := \ & \int_{\Sigma'} \left\{\boldsymbol{q}_t(\square) + \boldsymbol{u}(\cdot)\cdot\underline{\underline{\boldsymbol{\pi}}}_t(\square) + \boldsymbol{v}(\cdot)\cdot\underline{\underline{\boldsymbol{P}}}_t(\square)\right\} d^5\Sigma' - \\ & (\boldsymbol{u}\cdot\underline{\underline{\boldsymbol{\pi}}}_t)(\cdot) - (\boldsymbol{v}\cdot\underline{\underline{\boldsymbol{P}}}_t)(\cdot) + \\ & +\rho(\cdot)\Big\{\boldsymbol{v}(\cdot)\left(\boldsymbol{v}(\cdot)^2 - \boldsymbol{v}^2(\cdot)\right) + \frac{1}{2}\left(\boldsymbol{v}(\cdot)\boldsymbol{v}^2(\cdot) + (\boldsymbol{v}\boldsymbol{v}^2)(\cdot)\right) - \\ & (\boldsymbol{v}\boldsymbol{v})(\cdot)\cdot\boldsymbol{v}(\cdot) + \theta\Big[\boldsymbol{v}(\cdot)\left(\boldsymbol{\omega}(\cdot)^2 - \boldsymbol{\omega}^2(\cdot)\right) + \end{aligned} \tag{25}$$

$$\frac{1}{2}\left(\boldsymbol{v}(\cdot)(\boldsymbol{v}\boldsymbol{\omega})(\cdot)+(\boldsymbol{v}\boldsymbol{\omega}^2)(\cdot)\right)-(\boldsymbol{v}\boldsymbol{\omega})(\cdot)\cdot\boldsymbol{\omega}(\cdot)\Big]+$$

$$(\boldsymbol{v}\epsilon_t)(\cdot)-\boldsymbol{v}(\cdot)\epsilon(\cdot)\Big\}$$

$$\boldsymbol{Q}(\cdot) := \rho(\cdot)\boldsymbol{n}\times\Big\{\boldsymbol{u}(\cdot)\left(\boldsymbol{v}(\cdot)^2-\boldsymbol{v}^2(\cdot)\right)+\frac{1}{2}\left(\boldsymbol{u}(\cdot)\boldsymbol{v}^2(\cdot)+(\boldsymbol{u}\boldsymbol{v}^2)(\cdot)\right)-$$
$$(\boldsymbol{u}\boldsymbol{v})(\cdot)\cdot\boldsymbol{v}(\cdot)+\theta\Big[\boldsymbol{u}(\cdot)\left(\boldsymbol{\omega}(\cdot)^2-\boldsymbol{\omega}^2(\cdot)\right)+\frac{1}{2}\Big(\boldsymbol{u}(\cdot)\boldsymbol{\omega}^2(\cdot)+$$
$$+(\boldsymbol{u}\boldsymbol{\omega}^2)(\cdot)\Big)-(\boldsymbol{u}\boldsymbol{\omega})(\cdot)\cdot\boldsymbol{\omega}(\cdot)\Big]+(\boldsymbol{u}\epsilon_t)(\cdot)-\boldsymbol{u}(\cdot)\epsilon(\cdot)\Big\} \tag{26}$$

energy production:

$$r(\cdot) := \frac{1}{\rho(\cdot)}\int_{\Sigma'}\rho_t(\Box)[r_t(\Box)+\boldsymbol{k}_t(\Box)\cdot\boldsymbol{v}+\boldsymbol{g}_t(\Box)\cdot\boldsymbol{u}]\,d^5\Sigma' - \tag{27}$$
$$\boldsymbol{f}(\cdot)\cdot\boldsymbol{v}(\cdot)-\boldsymbol{g}(\cdot)\cdot\boldsymbol{u}(\cdot)\ .$$

A macroscopic director did not appear and was not defined up to now.

The position part Σ of the doubled phase space Ω is distinguished from the physical space IR^3 by the internal variable *n* of the microscopic director. For formulating balance equations on IR^3 we must get rid of the microscopic director without loosing the information due to orientation. The derivation of these usual balance equations including a set of equations describing the macroscopic orientation of the fluid can be found elsewhere.[14] The result is that these balance equations on IR^3 are the usual balances of a micropolar continuum,[5] but the essential difference is that all balanced quantities are statistically defined.

5 BALANCE EQUATIONS FOR ALIGNMENT TENSORS

We use the concept of alignment tensors[7] for a macroscopic description of the orientational distribution of the liquid crystal. The main idea of this approach is to expand the orientation distribution function $f(\cdot)$ into a series of multipoles

$$f(\cdot) := \frac{\rho(\cdot)}{\rho(\boldsymbol{x},t)} = \frac{1}{4\pi}\left(1+\sum_{l=1}^{\infty}(2l-1)!!a_{\mu_1\ldots\mu_l}(\boldsymbol{x},t)\,\overline{\hat{n}_{\mu_1}\cdots\hat{n}_{\mu_l}}\right)\ . \tag{28}$$

Here is

$$l!! = l(l-2)(l-4)\cdots\quad , \tag{29}$$

$\hat{\boldsymbol{n}}$ is a the unit vector

$$\hat{\boldsymbol{n}} := \|\boldsymbol{n}\|^{-1}\boldsymbol{n}\ , \tag{30}$$

greek indices $\mu_1, \ldots, \mu_l$ denote the components of a vector (general: a tensor) with respect to a cartesian basis and $\overline{}$ marks the (totally) symmetric irreducible part of a tensor, that means for a given tensor $b_{\mu_1\ldots\mu_l}$ is $\overline{b_{\mu_1\ldots\mu_l}}$ symmetric with respect to index permutations and will vanish for arbitrary contractions ($\overline{b_{\mu\mu\mu_3\ldots\mu_l}} = 0$).

The tensorial coefficients $a_{\mu_1\ldots\mu_l}$ in Equation (28) are called the alignment tensors of order l; they are given by

$$a_{\mu_1\ldots\mu_l}(\boldsymbol{x},t) := \frac{2l+1}{l!}\oint_{S^2} f(\cdot)\,\overline{\hat{n}_{\mu_1}\cdots\hat{n}_{\mu_l}}\;d^2n\ . \tag{31}$$

For deriving balance equations for the alignment tensors we first need an equation for the orientation distribution function $f(\cdot)$. Inserting the definition Equation (28) of $f(\cdot)$ into the mass balance per orientation Equation (10) we get after a brief calculation

$$\frac{\partial}{\partial t}f(\cdot) + \nabla_{\boldsymbol{x}}\cdot(\boldsymbol{v}(\cdot)f(\cdot)) + \boldsymbol{n}\cdot\nabla_{\boldsymbol{n}}\times(\boldsymbol{\omega}(\cdot)f(\cdot)) + f(\cdot)(\frac{\partial}{\partial t} + \boldsymbol{v}(\cdot)\cdot\nabla_{\boldsymbol{n}})\ln\rho(\boldsymbol{x},t) = 0. \tag{32}$$

Now we insert the multipole expansion Equation (28) of $f(\cdot)$ in Equation (32). With the help of an orthogonality relation[9] we are able to project out of Equation (32) a relaxation equation for the alignment tensor of k th order. This calculation is a rather lenghthy one[3] and will be published elsewhere.[6] As a result we obtain a system of coupled partial differential equations called the alignment tensor balance equations[14] which can be written down in a short form

$$\left(\frac{\partial}{\partial t} + \boldsymbol{v}(\boldsymbol{x},t)\cdot\nabla_{\boldsymbol{x}}\right)a_{\nu_1\cdots\nu_k} - k\left(\overline{\boldsymbol{\omega}(\boldsymbol{x},t)\times\underline{\boldsymbol{a}_k}}\right)_{\nu_1\cdots\nu_k} = \left\{\text{ all orders }\right\}. \tag{33}$$

The right hand side of Equation (33) which depends on alignment tensors of all orders has a typical form:

$$\left\{\text{ all orders }\right\} = \mathcal{F}[\delta\boldsymbol{v}(\cdot), \delta\boldsymbol{\omega}(\cdot)], \qquad \mathcal{F}[\mathrm{o},\mathrm{o}] = 0\ . \tag{34}$$

Here the peculiar velocities

$$\delta\boldsymbol{v}(\cdot) := \boldsymbol{v}(\cdot) - \boldsymbol{v}(\boldsymbol{x},t), \qquad \delta\boldsymbol{\omega}(\cdot) := \boldsymbol{\omega}(\cdot) - \boldsymbol{\omega}(\boldsymbol{x},t)\ . \tag{35}$$

are introduced.

The left hand side of Equation (33) is Jaumann's total time derivative for symmetric irreducible tensors. Therefore that side of the equation describes the changes of the alignment tensors which can be observed from a frame transferred with

$$\boldsymbol{v}(\boldsymbol{x},t) := \int_{S^2}\boldsymbol{v}(\cdot)f(\cdot)\,d^2n \tag{36}$$

and rotated with

$$\boldsymbol{\omega}(\boldsymbol{x},t) := \int_{S^2}\boldsymbol{\omega}(\cdot)f(\cdot)\,d^2n\ . \tag{37}$$

Thus the right hand side of Equation (33) is due to the production of alignment. This production of course will vanish, if there are no deviations in the velocity distribution of $v(\cdot)$ and $\omega(\cdot)$ from their averages $v(x, t)$ and $\omega(x, t)$. This will be the case, if the orientation-diffusion (differently orientated molecules have different velocities) and the orientation-relaxation (differently orientated molecules have different angular velocities) are finished. The special form of the alignment production involves generally all the alignment tensors of any order. A subdynamic even of the alignment tensor of second order will not exist in general. Nevertheless we suppose that the constitutive equations will suppress the influence of the higher rank tensors due to their faster orientation-relaxation.

If a special diffusion ansatz as constitutive equation is made in the position part of the doubled phase space

$$\rho(\cdot)\boldsymbol{v}(\cdot) = -D(\boldsymbol{x},t)\nabla_x\rho(\cdot) \ , \tag{38}$$

$$f(\cdot)\boldsymbol{u}(\cdot) = -\Omega(\boldsymbol{x},t)\nabla_n f(\cdot) \ , \tag{39}$$

we get a relatively easy balance equation for the alignment tensor of order k

$$\begin{aligned} &\frac{\partial}{\partial t}\underline{\boldsymbol{a}}_k(\boldsymbol{x},t) - D(\boldsymbol{x},t)\nabla_x\cdot\nabla_x\underline{\boldsymbol{a}}_k(\boldsymbol{x},t) + k(k+1)\Omega(\boldsymbol{x},t)\underline{\boldsymbol{a}}_k(\boldsymbol{x},t) = \\ &= \nabla_x D(\boldsymbol{x},t)\cdot\nabla_x\underline{\boldsymbol{a}}_k(\boldsymbol{x},t) + 2D(\boldsymbol{x},t)\nabla_x\underline{\boldsymbol{a}}_k(\boldsymbol{x},t)\cdot\nabla_x \ln\rho(\boldsymbol{x},t) \end{aligned} \tag{40}$$

which does not couple to alignment tensors of other orders.[8,10]

6 CLOSURE

Starting out with statistically founded global balance equations formulated on the doubled phase space (position and orientation) we get local balance equations for mass, momentum, spin, and internal energy on the position part of this doubled phase space including the microscopic director as variable. Expansion of the distribution function concerning the orientations of the microscopic directors yields an alignment tensor balance. Its production term disappears with vanishing orientation-diffusion and orientation-relaxation. Diffusion ansatzes as constitutive equations yield a simplified alignment tensor balance.

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