Mesoscopic Interpretation of Fokker-Planck Equation Describing Time Behavior of Liquid Crystal Orientation

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Abstract

Starting out with the mesoscopic mass balance for liquid crystals we derive the balance equation for the orientation distribution function (ODF) of the molecules which is of Fokker-Planck type. Comparison of this mesoscopic generated Fokker-Planck equation to well-known statistically induced balance equations of the ODF results in a slip relation between the rotation of the liquid crystal and the angular velocity of molecules of different orientations. The difference between these two angular velocities is caused by the torque of the meanfield, by the velocity gradient, by the alignment, and by the non-isotropy of the ODF.

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1 Introduction

Liquid crystals are phases showing an orientational order of molecules which are of elongated or of plane shape, so that an orientational order of them can

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be defined. The molecules themselves may be uniaxial (i.e. their alignment can be described by one direction) or biaxial (for which two axes are necessary to fix their orientation). The orientation of a single uniaxial molecule is described by a unit vector $\boldsymbol{n}$ -called *microscopic director*- pointing into the rotation symmetry axis of the molecule. Because of thermal fluctuations the molecules are not totally aligned, but we have a distribution function $f(\boldsymbol{n}, \boldsymbol{x}, t)$ describing the orientation of the molecules at time t and position $\boldsymbol{x}$, called *orientation distribution function* (ODF). Besides the orientational order an additional spatial order of the centers of mass of the molecules is possible which causes a great variety of liquid crystal phases.

The *mesoscopic concept* describing liquid crystals introduces the above mentioned microscopic director as a variable which is related to the orientation of one rigid particle only. The anisotropic fluid can be formally treated as a mixture by regarding all particles of a volume element having the same orientation as one component of the fluid [1]. Thus the ODF results as the fraction of the mass density of one component over the mass density of the mixture. Because mixture theory is well developed [2] balance equations for liquid crystals can be written down very easily by use of this method. The domain on which these balances are defined differs from the usual one by the microscopic director which is introduced as an additional variable.

In the kinetic theory of liquid crystals equations of motion for the ODF are well-known in case of homogeneous alignment, that means, if the ODF is independent of the position $f(\boldsymbol{n}, t)$. These equations are of Fokker-Planck type [3, 4]. On the other side we know from the mesoscopic theory of liquid crystals a differential equation for the ODF [5], called *mesoscopic Fokker-Planck equation*. Aim of this paper is to compare this mesoscopic Fokker-Planck equation with the statistically induced Fokker-Planck equations of the kinetic theory of liquid crystals.

For this comparison we have to get rid of the position in the mesoscopic Fokker-Planck equation by introducing *uniform systems*. Then we derive an expression for the mesoscopic angular velocity of the molecules in terms of the ODF, the alignment tensor, the diffusion constant, the velocity gradient, and the external torque potential. Thus a statistical interpretation of the mesoscopic angular velocity of the molecules is possible, and on the other side the statistical Fokker-Planck equations for homogeneous alignment appear as a special case of the mesoscopic Fokker-Planck equation which is induced by the phenomenological continuum theory of liquid crystals.

2 Fokker-Planck equations for homogeneous alignment

In the kinetic theory of liquid crystals two forms of the equation of motion for the ODF of the molecules are used [3, 4]

$$\partial_t f(\boldsymbol{n},t) - D\boldsymbol{L}\cdot\left[\boldsymbol{L}f + \frac{1}{kT} f\boldsymbol{L}(H(\boldsymbol{n}) + U^{ex})\right] + \\ + \boldsymbol{L}\cdot\boldsymbol{n}\times(\nabla\boldsymbol{V}\cdot\boldsymbol{n}f) = 0, \qquad (1)$$

and

$$\partial_t f(\boldsymbol{n},t) + \boldsymbol{\Omega}^*\cdot\boldsymbol{L}f - \\ -D\boldsymbol{L}\cdot\left[\boldsymbol{L}f - f\boldsymbol{L}(\frac{T^*}{T}\mathbf{a} + \frac{\kappa}{6D}\overline{\nabla\boldsymbol{V}}\,) : \overline{\boldsymbol{n}\boldsymbol{n}}\right] = 0. \qquad (2)$$

Here $f(\boldsymbol{n},t)$ is the ODF for the microscopic director $\boldsymbol{n}$ which is defined as a unit vector pointing into the direction of the axis of a uniaxial elongated molecule or being perpendicular to the plane in which a disc-like molecule is located. Because the ODF is independent of the position only homogeneous alignment can be described. D is a diffusion constant, $\boldsymbol{L}$ is a differential operator defined by

$$\boldsymbol{L} = \boldsymbol{n}\times\partial_{\boldsymbol{n}}, \qquad (3)$$

$H(\boldsymbol{n})$ is the meanfield potential and U^{ex} the potential of the external field. The gradient of the material velocity $\boldsymbol{V}$ is presupposed to be constant, that means to be independent of position $\boldsymbol{x}$ (homogeneous alignment) and orientation $\boldsymbol{n}$. The angular velocity $\boldsymbol{\Omega}^*$ due to the motion of the fluid is defined by

$$2\boldsymbol{\Omega}^*(t) := \varepsilon : \boldsymbol{\Omega}(t), \\ 2\boldsymbol{\Omega}(t) = \varepsilon\cdot 2\boldsymbol{\Omega}^*(t) := \nabla\boldsymbol{V} - (\nabla\boldsymbol{V})^\top. \qquad (4)$$

Here ε is the Levi-Civita tensor. The characteristic temperature T^* in (2) is proportional to the critical temperature of the phase transition nematic-isotropic[1], whereas T denotes the actual temperature of the nematic phase.

[1]According to [6] $T^* = (15/2)T_{crit}$.

The meanfield potential in (1) associated with the molecular alignment is given by [6]

$$H = -kT^{*}\mathbf{a} : \overline{\boldsymbol{n}\boldsymbol{n}}. \tag{5}$$

Here the alignment tensor (of second order) is defined by

$$\mathbf{a} := \int_{S^2} f(\boldsymbol{n}, t)\, \overline{\boldsymbol{n}\boldsymbol{n}}\, d^2 n. \tag{6}$$

The hook $\overline{}$ characterizes the symmetric and traceless dyadic product, and κ in (2) is a molecular parameter depending on the viscosity of the fluid and on the ratio of the semi-axes of the molecule along and perpendicular to $\boldsymbol{n}$. According to [4] different values of κ, $\kappa > 0$, $\kappa < 0$ and $\kappa = 0$, describe prolate, oblate, and spherical molecules. Of course (1) and (2) are not independent of each other. As it is performed in the appendix (A) the equations (1) and (2) are equal, if $U^{ex} = 0$ and $\kappa = 3$.

The background of the Fokker-Planck equations (1) and (2) is of statistical nature. Transition probabilities between the different orientations of the molecules are presupposed so that the resulting stochastic Markovian process obeys the Chapman-Kolmogorov equations for the transition probabilities. If there is an initial condition for the ODF, these transition probabilities transform it to its actual configuration. The statistical presuppositions made for the process and its ODF represent the model by which the dynamics of the orientation of the molecules in a liquid crystal is described. From a more phenomenological point of view the Fokker-Planck equations (1) and (2) are ad-hoc equations for orientation dynamics.

The question now arises, if there is any phenomenological interpretation of (1) and (2). Because (1) and (2) are equations of motion of the ODF a phenomenological interpretation can only be found on a mesoscopic level, that means, on a level which includes the ODF, but which is not of statistical nature. Such a mesoscopic level is well developed for liquid crystals [1, 5, 7], [8] which can be described by orientational balances. These are balances defined on the so-called *nematic space* which includes beyond position and time the orientation represented by $\boldsymbol{n}$ as a variable . Starting out with the orientational mass balance, a balance of the ODF can be achieved which we will compare with (1) and (2) in section 5 and by which we can interpret (1) and (2) mesoscopically.

3 Differential equation of orientation distribution function

The differential equation for the orientation distribution function of the molecules can be derived within the frame of the mesoscopic theory of liquid crystals [5, 9]. In the mesoscopic theory a liquid crystal can be considered as a mixture of differently orientated uniaxial molecules which can be modelled by ellipsoids whose figure axes correspond to the direction of the microscopic director $\boldsymbol{n}$. All these unit vectors of different orientation span the unit sphere. The ODF $f(\boldsymbol{n}, \boldsymbol{x}, t)$ defined on this unit sphere describes, at position $\boldsymbol{x}$ (of a volume element) and time t, the fraction of those molecules pointing into the direction of $\boldsymbol{n}$ which can be considered as a special component (with a "continuous" component index $\boldsymbol{n}$) of a mixture. Because mixture theory is well developed [2], it is easy to derive so-called orientational balance equations [1]. These equations are defined on the so-called *nematic space* spanned by $(\boldsymbol{n}, \boldsymbol{x}, t) \in S^2 \times R^3 \times R^1$. Thus also the mesoscopic ODF is defined on the nematic space

$$f(\boldsymbol{n}, \boldsymbol{x}, t) \equiv f(\cdot), \qquad (\cdot) \equiv (\boldsymbol{n}, \boldsymbol{x}, t) \in S^2 \times R^3 \times R^1. \tag{7}$$

In order to obtain the differential equation of the ODF the *orientation mass density* $\varrho(\boldsymbol{n}, \boldsymbol{x}, t)$ is introduced which describes the density of all those molecules in a volume element whose axes point in the direction of $\boldsymbol{n}$. The usual mass density $\varrho(\boldsymbol{x}, t)$ of the liquid crystal is related to the orientational one $\varrho(\cdot)$ by integrating over all orientations

$$\varrho(\boldsymbol{x}, t) = \int_{S^2} \varrho(\cdot) d^2 n. \tag{8}$$

Because of its normalization the ODF itself is defined by

$$f(\cdot) := \frac{\varrho(\cdot)}{\varrho(\boldsymbol{x}, t)}, \qquad \int_{S^2} f(\cdot) d^2 n = 1, \quad \text{for all } (\boldsymbol{x}, t). \tag{9}$$

To obtain the local form of the orientational balance equations on the nematic space we need a modified Reynolds transport theorem [5]

$$\frac{d}{dt} \int_{G(t)} \int_{g(t)} \qquad \Phi(\cdot) d^2 n d^3 x =$$

$$= \int_{G(t)} \int_{g(t)} \qquad [\partial_t \Phi(\cdot) + \nabla_x \cdot (\boldsymbol{v}_M \Phi(\cdot)) + \\ + \nabla_n \cdot (\boldsymbol{u}_M \Phi(\cdot))] \, d^2n d^3x. \tag{10}$$

Here $\boldsymbol{v}_M$ and $\boldsymbol{u}_M$ are the velocities of mapping, i.e. the velocities of $G(t) \in R^3$ and $g(t) \in S^2$ which are not material velocities in case of open systems. If $\boldsymbol{v}_M \equiv 0$, and Φ and $\boldsymbol{u}_M$ are independent of $\boldsymbol{x}$ Reynolds transport theorem (10) reads

$$\frac{d}{dt} \int_{g(t)} \Phi(\boldsymbol{n}, t) d^2n = \\ = \int_{g(t)} [\partial_t \Phi(\boldsymbol{n}, t) + \nabla_n \cdot (\boldsymbol{u}_M \Phi(\boldsymbol{n}, t))] \, d^2n. \tag{11}$$

From (10) we obtain the mass balance per orientation [5]

$$\partial_t \varrho(\cdot) + \nabla_x \cdot (\boldsymbol{v} \varrho(\cdot)) + \nabla_n \cdot (\boldsymbol{u} \varrho(\cdot)) = 0. \tag{12}$$

Here $\boldsymbol{v}$ is the material velocity, and $\boldsymbol{u}$ is the orientation change velocity perpendicular to $\boldsymbol{n}$ which corresponds to the angular velocity of the molecules

$$\boldsymbol{n} \cdot \boldsymbol{u}(\cdot) = 0, \qquad \boldsymbol{\omega}(\cdot) := \boldsymbol{n} \times \boldsymbol{u}(\cdot). \tag{13}$$

Inserting $(9)_1$ the orientational mass balance (12) results after a brief calculation in

$$\partial_t f(\cdot) + \nabla_x \cdot [\boldsymbol{v}(\cdot) f(\cdot)] + \\ + \nabla_n \cdot [\boldsymbol{u}(\cdot) f(\cdot)] + f(\cdot)[\partial_t + \boldsymbol{v}(\cdot) \cdot \nabla_x] ln \varrho(\boldsymbol{x}, t) = 0. \tag{14}$$

This balance equation of the ODF is derived on the mesoscopic level of description. It is defined on the nematic space, and therefore it is more general than (1) and (2) which do not include the position $\boldsymbol{x}$. The last term in (14) contains the total mass density $\varrho(\boldsymbol{x}, t)$ which therefore influences the time rate of the ODF.

The aim of the paper is to compare (1) and (2) to (14) thus giving a mesoscopic interpretation of the statistically introduced Fokker-Planck equations (1) and (2). For this purpose the dependence of the position of (14) has to be eliminated, what will be done in the next section.

4 Uniform systems

More than one decade ago differential equations of Fokker-Planck type for the orientation of uniaxial molecules have been proposed [3, 4]. For comparing these equations to the differential equation of the mesoscopic ODF (14) we have to get rid of the position because (1) and (2) do not contain it, although a velocity gradient appears. Consequently (1) and (2) do not describe homogeneous systems because for these also $\nabla \boldsymbol{V}$ would vanish. Therefore we introduce the concept of *uniform systems* which is defined by integrating over the position part of the nematic space. Thus all quantities of a uniform system are defined on $S^2 \times R^1$. The mass density and the ODF become

$$\varrho(\boldsymbol{n}, t) := \int_{G(t)} \varrho(\cdot) d^3x, \tag{15}$$

$$f(\boldsymbol{n}, t) := \frac{\varrho(\boldsymbol{n}, t)}{M_{G(t)}}, \qquad M_{G(t)} := \int_{S^2} \int_{G(t)} \varrho(\cdot) d^3x d^2n. \tag{16}$$

Here $M_{G(t)}$ is the total mass of the system, and $f(\boldsymbol{n}, t)$ is normalized

$$\int_{S^2} f(\boldsymbol{n}, t) d^2n = 1. \tag{17}$$

For obtaining the mass balance in a uniform system we integrate (12) over the positions and use (15)

$$\partial_t \varrho(\boldsymbol{n}, t) \ + \ \oint_{\partial G(t)} d\boldsymbol{f} \cdot \boldsymbol{v}(\cdot) \varrho(\cdot) \ + \\ + \nabla_n \cdot \int_{G(t)} \boldsymbol{u}(\cdot) \varrho(\cdot) d^3x = 0. \tag{18}$$

If the momentum of the system is conserved, and if we define

$$\boldsymbol{u}(\boldsymbol{n}, t) \varrho(\boldsymbol{n}, t) := \int_{G(t)} \boldsymbol{u}(\cdot) \varrho(\cdot) d^3x, \tag{19}$$

(18) results in the mass balance of a uniform system

$$\partial_t \varrho(\boldsymbol{n}, t) \ + \ \nabla_n \cdot \boldsymbol{u}(\boldsymbol{n}, t) \varrho(\boldsymbol{n}, t) = 0. \tag{20}$$

According to $(16)_1$ the differential equation of the ODF in orientation space is

$$\partial_t f(\boldsymbol{n},t) \ + \ \nabla_n \cdot [\boldsymbol{u}(\boldsymbol{n},t) f(\boldsymbol{n},t)] = 0. \tag{21}$$

From (13) follows immediately

$$\int_{G(t)} \varrho(\cdot)\boldsymbol{\omega}(\cdot) d^3x = \boldsymbol{n} \times \int_{G(t)} \varrho(\cdot)\boldsymbol{u}(\cdot) d^3x, \tag{22}$$

which with the definition

$$\varrho(\boldsymbol{n},t)\boldsymbol{\omega}(\boldsymbol{n},t) := \int_{G(t)} \varrho(\cdot)\boldsymbol{\omega}(\cdot) d^3x \tag{23}$$

results in the angular velocity of the molecules with respect to the observer in orientation space

$$\boldsymbol{\omega}(\boldsymbol{n},t) = \boldsymbol{n} \times \boldsymbol{u}(\boldsymbol{n},t). \tag{24}$$

According to $(13)_2$ and (19) we obtain

$$\int_{G(t)} \boldsymbol{n} \cdot \varrho(\cdot)\boldsymbol{u}(\cdot) d^3x \ = \ 0 \ = \ \boldsymbol{n} \cdot \varrho(\boldsymbol{n},t)\boldsymbol{u}(\boldsymbol{n},t), \tag{25}$$

and consequently (24) yields

$$\boldsymbol{n} \times \boldsymbol{\omega}(\boldsymbol{n},t) \ = \ -\boldsymbol{u}(\boldsymbol{n},t). \tag{26}$$

Inserting (26) into (21) results in the mesoscopically founded differential equation of Fokker-Planck type for the ODF on orientation space in uniform systems

$$\partial_t f(\boldsymbol{n},t) \ + \ \nabla_n \cdot [\boldsymbol{\omega}(\boldsymbol{n},t) \times \boldsymbol{n} f(\boldsymbol{n},t)] = 0. \tag{27}$$

As in appendix (B) is demonstrated

$$\nabla_n \cdot [\boldsymbol{\omega}(\boldsymbol{n},t) \times \boldsymbol{n} f(\boldsymbol{n},t)] = \boldsymbol{L} \cdot [\boldsymbol{\omega}(\boldsymbol{n},t) f(\boldsymbol{n},t)] \tag{28}$$

is valid. Consequently the mesoscopic Fokker-Planck equation in uniform systems (27) becomes

$$\partial_t f(\boldsymbol{n},t) \ + \ \boldsymbol{L} \cdot [\boldsymbol{\omega}(\boldsymbol{n},t) f(\boldsymbol{n},t)] = 0. \tag{29}$$

5 Comparison of statistical and mesoscopic Fokker-Planck equations

We now compare the mesoscopic Fokker-Planck equation (29) to the statistical ones (1) and (2). For that purpose we transform (46), derived in appendix A, into the following shape:

$$\partial_t f(\boldsymbol{n},t) + \boldsymbol{L}\cdot f\,[\boldsymbol{\Omega}^* - D\boldsymbol{L} lnf + \\ +\boldsymbol{L}(D\frac{T^*}{T}\mathbf{a} + \frac{1}{2}\overline{\nabla\boldsymbol{V}}\,) : \overline{\boldsymbol{n}\boldsymbol{n}} - \frac{D}{kT}\boldsymbol{L}U^{ex}\Big] = 0. \tag{30}$$

Comparison with (29) results in the rotational angular velocity (24) of the molecules

$$\boldsymbol{\omega}(\boldsymbol{n},t) = \boldsymbol{\Omega}^* - \\ -D\boldsymbol{L}\left[lnf - (\frac{T^*}{T}\mathbf{a} + \frac{1}{2D}\overline{\nabla\boldsymbol{V}}\,) : \overline{\boldsymbol{n}\boldsymbol{n}} - \frac{1}{kT}\boldsymbol{L}U^{ex}\right]. \tag{31}$$

Consequently we obtain for the difference between the angular velocity of the fluid and that of the molecules (the so-called *slip*)

$$\boldsymbol{\Omega}^* - \boldsymbol{\omega}(\boldsymbol{n},t) = \\ = D\boldsymbol{L}\left[lnf - (\frac{T^*}{T}\mathbf{a} + \frac{1}{2D}\overline{\nabla\boldsymbol{V}}\,) : \overline{\boldsymbol{n}\boldsymbol{n}} - \frac{1}{kT}\boldsymbol{L}U^{ex}\right]. \tag{32}$$

The two angular velocities $\boldsymbol{\Omega}^*$ and $\boldsymbol{\omega}(\boldsymbol{n},t)$ are independent of each other: According to (4) $\boldsymbol{\Omega}^*$ belongs to the macroscopic rotation of the fluid, whereas the orientation dependent $\boldsymbol{\omega}(\boldsymbol{n},t)$ is due to the mesoscopic rotation of the molecules. Because the slip is a difference of angular velocities, it is independent of the observer. Therefore the rotational angular velocity becomes in a co-rotational frame ($\boldsymbol{\Omega}^* = \mathbf{0}$)

$$\boldsymbol{\omega}^{corot}(\boldsymbol{n},t) = \\ -D\boldsymbol{L}\left[lnf - (\frac{T^*}{T}\mathbf{a} + \frac{1}{2D}\overline{\nabla\boldsymbol{V}}\,) : \overline{\boldsymbol{n}\boldsymbol{n}} - \frac{1}{kT}\boldsymbol{L}U^{ex}\right]. \tag{33}$$

6 Results

As we can see from (32) there are three reasons for the slip of the molecules in a rotational motion of the liquid crystal: The ODF f is not isotropic (it depends on $\boldsymbol{n}$), the alignment tensor $\mathbf{a}$ and/or the velocity gradient $\nabla \boldsymbol{V}$ do not vanish, and the external potential U^{ex} depends on $\boldsymbol{n}$. Thus we obtain an interpretation of the mesoscopic quantity $\boldsymbol{\omega}(\boldsymbol{n}, t)$ by (31): It depends on the ODF, on the alignment tensor, on the symmetric traceless part of the velocity gradient, and on the external potential. On the other side we obtain a novel mesoscopic interpretation of the statistical Fokker-Planck equations (1) and (2) by (29) and (31): The square bracket in (30) is just proportional to the slip, and the statistically founded Fokker-Planck equations are compatible with the mesoscopically derived differential equation of the ODF in case of uniform systems. Consequently the statistical Fokker-Planck equations (1) and (2) appear as a special case of the mesoscopic Fokker-Planck equation (29), if the slip between the angular velocities of the fluid and the molecules is given by (32). Hence statistically founded Fokker-Planck equations fit into the mesoscopic theory which is governed by orientational balances.

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Appendix

A

Inserting (5) into (1) we obtain

$$\partial_t f(\boldsymbol{n}, t) - D\boldsymbol{L} \cdot \left[\boldsymbol{L} f - f \boldsymbol{L} \left(\frac{T^*}{T} \mathbf{a} : \overline{\boldsymbol{n}\boldsymbol{n}} - \frac{1}{kT} U^{ex} \right) \right] + \\ + \boldsymbol{L} \cdot \boldsymbol{n} \times (\nabla \boldsymbol{V} \cdot \boldsymbol{n} f) = 0. \qquad (34)$$

By use of (4) we have

$$\nabla \boldsymbol{V} = 2\boldsymbol{\Omega} + (\nabla \boldsymbol{V})^{\top} = \boldsymbol{\Omega} + \overline{\nabla \boldsymbol{V}} + \left(\frac{1}{3} Tr \nabla \boldsymbol{V}\right) \mathbf{1}, \tag{35}$$

and therefore

$$\boldsymbol{n} \times (\nabla \boldsymbol{V} \cdot \boldsymbol{n}) = \boldsymbol{n} \times (\overline{\nabla V} \cdot \boldsymbol{n}) + \boldsymbol{n} \times (\boldsymbol{\Omega} \cdot \boldsymbol{n}) \tag{36}$$

and

$$\begin{aligned} &\boldsymbol{L} \cdot [\boldsymbol{n} \times (\nabla \boldsymbol{V} \cdot \boldsymbol{n}) f] = \\ &= \boldsymbol{L} \cdot [\boldsymbol{n} \times (\overline{\nabla \boldsymbol{V}} \cdot \boldsymbol{n}) f] + \boldsymbol{L} \cdot [\boldsymbol{n} \times (\boldsymbol{\Omega} \cdot \boldsymbol{n}) f] \end{aligned} \tag{37}$$

are valid. By use of $(4)_2$ the last term of (36) yields

$$\begin{aligned} &\boldsymbol{n} \times (\boldsymbol{\Omega} \cdot \boldsymbol{n}) = \boldsymbol{n} \times (\epsilon : \boldsymbol{\Omega}^{*} \boldsymbol{n}) = \\ &= \boldsymbol{n} \times (\boldsymbol{\Omega}^{*} \times \boldsymbol{n}) = \boldsymbol{\Omega}^{*} - \boldsymbol{n}(\boldsymbol{\Omega}^{*} \cdot \boldsymbol{n}). \end{aligned} \tag{38}$$

Therefore the last term of (37) results in

$$\boldsymbol{L} \cdot [\boldsymbol{n} \times (\boldsymbol{\Omega} \cdot \boldsymbol{n}) f] = \boldsymbol{L} \cdot \boldsymbol{\Omega}^{*} f - \boldsymbol{L} \cdot \boldsymbol{n}(\boldsymbol{\Omega}^{*} \cdot \boldsymbol{n}) f. \tag{39}$$

Here the last term vanishes using (3)

$$\begin{aligned} &[\boldsymbol{n} \times \partial_{\boldsymbol{n}}] \cdot \boldsymbol{n}(\boldsymbol{\Omega}^{*} \cdot \boldsymbol{n}) f = \boldsymbol{n} \cdot [\partial_{\boldsymbol{n}} \times \boldsymbol{n}(\boldsymbol{\Omega}^{*} \cdot \boldsymbol{n}) f] = \\ &= \boldsymbol{n} \cdot (\boldsymbol{\Omega}^{*} \cdot \boldsymbol{n}) f \partial_{\boldsymbol{n}} \times \boldsymbol{n} + \boldsymbol{n} \cdot [\partial_{\boldsymbol{n}} (\boldsymbol{\Omega}^{*} \cdot \boldsymbol{n}) f \times \boldsymbol{n}] = 0. \end{aligned} \tag{40}$$

Therefore (37) yields by use of (39) and (40)

$$\boldsymbol{L} \cdot [\boldsymbol{n} \times (\nabla \boldsymbol{V} \cdot \boldsymbol{n}) f] = \boldsymbol{L} \cdot [\boldsymbol{n} \times (\overline{\nabla \boldsymbol{V}} \cdot \boldsymbol{n}) f] + \boldsymbol{L} \cdot \boldsymbol{\Omega}^{*} f. \tag{41}$$

For transforming the first term of the right-hand side of (41) we consider

$$\boldsymbol{L}[\overline{\nabla \boldsymbol{V}} : \overline{\boldsymbol{n}\boldsymbol{n}}] = \boldsymbol{L}[\overline{\nabla \boldsymbol{V}} : \boldsymbol{n}\boldsymbol{n}] = (\boldsymbol{n} \times \partial_{\boldsymbol{n}})[\overline{\nabla \boldsymbol{V}} : \boldsymbol{n}\boldsymbol{n}]. \tag{42}$$

In components we obtain, if $\boldsymbol{V}$ does not depend on the orientation $\boldsymbol{n}$

$$\begin{aligned} &\varepsilon_{ijk} n_j \partial_{n_k} (\overline{\nabla \boldsymbol{V}})_{rs} n_r n_s = \varepsilon_{ijk} n_j (\overline{\nabla \boldsymbol{V}})_{rs} (\delta_{kr} n_s + n_r \delta_{ks}) = \\ &= (\overline{\nabla \boldsymbol{V}})_{rs} n_j (\varepsilon_{ijr} n_s + \varepsilon_{ijs} n_r) = \\ &= \varepsilon_{ijr} n_j [(\overline{\nabla \boldsymbol{V}})_{rs} n_s + (\overline{\nabla \boldsymbol{V}})_{sr} n_s]. \end{aligned} \tag{43}$$

Thus (42) results in

$$\boldsymbol{L}[\,\overline{\nabla \boldsymbol{V}}\,:\,\overline{\boldsymbol{n}\boldsymbol{n}}\,] = 2\boldsymbol{n} \times (\,\overline{\nabla \boldsymbol{V}}\,\cdot \boldsymbol{n}), \tag{44}$$

and

$$\boldsymbol{L} \cdot [\boldsymbol{n} \times (\,\overline{\nabla \boldsymbol{V}}\,\cdot \boldsymbol{n})f] = (1/2)\boldsymbol{L} \cdot f\boldsymbol{L}[\,\overline{\nabla \boldsymbol{V}}\,:\,\overline{\boldsymbol{n}\boldsymbol{n}}\,]. \tag{45}$$

Inserting this into (41) and (34) we obtain, if we take into consideration that $\boldsymbol{\Omega}^*$ does not depend on the orientation

$$\begin{aligned} &\partial_t f(\boldsymbol{n},t) + \boldsymbol{\Omega}^* \cdot \boldsymbol{L}f - D\boldsymbol{L} \cdot \Big[\boldsymbol{L}f \\ &-f\boldsymbol{L}(\frac{T^*}{T}\mathbf{a} + \frac{1}{2D}\,\overline{\nabla \boldsymbol{V}}\,) : \overline{\boldsymbol{n}\boldsymbol{n}} + \frac{1}{kT} f\boldsymbol{L}U^{ex}\Big] = 0. \end{aligned} \tag{46}$$

Consequently (46) and (2) are equal, if $U^{ex} = 0$ and $\kappa = 3$. Thus because of (34) also (1) and (2) are equal in this case.

B

Differentiation to the unit vector $\boldsymbol{n}$ is defined by the covariant derivative

$$\nabla_n := \partial_{\boldsymbol{n}} - \boldsymbol{n}(\boldsymbol{n} \cdot \partial_{\boldsymbol{n}}). \tag{47}$$

This yields

$$\nabla_n \times \boldsymbol{n} = \partial_{\boldsymbol{n}} \times \boldsymbol{n} - \boldsymbol{n}(\boldsymbol{n} \cdot \partial_{\boldsymbol{n}}) \times \boldsymbol{n} = 0 - \boldsymbol{n} \times (\boldsymbol{n} \cdot \partial_{\boldsymbol{n}})\boldsymbol{n} = 0. \tag{48}$$

The left-hand side of (28) is

$$\begin{aligned} \nabla_n \cdot [\boldsymbol{\omega}(\boldsymbol{n},t) \times \boldsymbol{n}f(\boldsymbol{n},t)] \equiv \nabla_n \cdot [f\boldsymbol{\omega} \times \boldsymbol{n}] = \\ = \boldsymbol{n} \cdot (\nabla_n \times f\boldsymbol{\omega}) - f\boldsymbol{\omega} \cdot (\nabla_n \times \boldsymbol{n}) = \boldsymbol{n} \cdot (\nabla_n \times f\boldsymbol{\omega}) = \\ = \boldsymbol{n} \times \nabla_n \cdot f\boldsymbol{\omega} = \boldsymbol{n} \times \partial_{\boldsymbol{n}} \cdot f\boldsymbol{\omega} = \boldsymbol{L} \cdot f\boldsymbol{\omega}. \end{aligned} \tag{49}$$

Here in the last two equations (47) and (3) were used. Thus (28) is proved.

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