On the Unified Theory for Non-Equilibrium Phenomena in the Isotropic and Nematic Phases of a Liquid Crystal; Spatially Inhomogeneous Alignment

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A nonlinear equation is derived which describes the relaxation of the alignment and the flow alignment in the isotropic and nematic phases of a liquid crystal. In addition to the previously treated case, contributions associated with spatial derivatives of the alignment are taken into account which stem from gradient terms occuring in the free energy (elastic energy) and from the flux of the alignment. Some applications are discussed. In particular, the Leslie and Frank coefficients of the nematic phase are expressed in terms of the equilibrium alignment order parameter and coefficients which are meaningful in both phases.

In this article, it is indicated how the previously developed unified theory [1] for nonequilibrium processes in the isotropic and nematic phases of a liquid crystal can be extended to the case where the alignment is spatially inhomogeneous. Two modifications have to be introduced. Firstly, in the free energy, terms containing spatial derivatives of the alignment have to be taken into account which are linked with the elastic energy. In as much as the phenomenological theory of Ref. [1] can be looked upon as a dynamic Landau theory, this extension can be referred to a dynamic Ginzburg-Landau theory. Secondly, however, a term containing the divergence of the flux of the alignment has to be included in the equation of change of the alignment tensor. A constitutive law which links this flux with the gradient of the alignment is set up by the standard procedure of irreversible thermodynamics. In the nonlinear relaxation equation for the alignment tensor, spatial derivatives up to 4-th order are taken into account. In the presence of a viscous flow, additional terms occur which are associated with flow birefringence and flow alignment. The equation is applicable to both the isotropic and nematic phases. For temperatures which are not too close to the temperature where the transition from the isotropic to the nematic phase takes place, the (inhomogeneous) relaxation equation can be linearized about the appropriate zero and nonzero equilibrium value of the alignment. It is briefly indicated how some well-known results for the isotropic and nematic phases are obtained as special cases of the unified theory. In particular, the Frank elasticity coefficient K and the Leslie coefficients γ_1, γ_2 are related to the order parameter and expressed in terms of coefficients which are meaningful in both phases.

1. Alignment Tensor

Here, we are only concerned with molecular orientation phenomena which are linked with the 2nd rank alignment tensor [1] $\mathbf{a}$. For a liquid of (effectively) axisymmetric particles one has, in Cartesian component notation [2],

$$a_{\mu\nu} \sim \langle \overline{u_\mu u_\nu} \rangle , \qquad (1)$$

where $\boldsymbol{u}$ is a unit vector parallel to the figure axis of a molecule. The bracket $\langle \ldots \rangle$ indicates an average over the molecules in the liquid. The symbol $\overline{\cdots}$ refers to the symmetric traceless part of a tensor, in particular, $\overline{u_\mu u_\nu} = u_\mu u_\nu - \frac{1}{3}\delta_{\mu\nu}$. The quantity $\mathbf{a}$ is associated with the optical anisotropy (birefringence) of a liquid and it is the most relevant type of alignment for a liquid crystal [3].

For a streaming liquid with flow velocity field $\boldsymbol{v}$, the equation of change of the alignment tensor can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t} a_{\mu\nu} - 2\, \overline{\varepsilon_{\mu\lambda\varkappa}\, \omega_\lambda\, a_{\varkappa\nu}} + \nabla_\lambda b_{\lambda,\mu\nu} = \left(\frac{\delta a_{\mu\nu}}{\delta t} \right)_{\mathrm{irr}} . \qquad (2)$$

Here $\dfrac{\mathrm{d}}{\mathrm{d}t} \equiv \dfrac{\partial}{\partial t} + v_\lambda \nabla_\lambda$ is the substantial derivative. The quantity $b_{\lambda,\mu\nu}$ is the flux of the alignment and

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$(\delta a_{\mu\nu}/\delta t)_{\mathrm{irr}}$ stands for the change of $\mathbf{a}$ associated with irreversible processes (relaxation, coupling with transport processes). The 2nd term in Eq. (2) describes the rotational motion of the molecules with an angular velocity

$$\boldsymbol{\omega} = \tfrac{1}{2}\,\mathrm{rot}\,\boldsymbol{v} \tag{3}$$

caused by the local rotation of the velocity field. For $\boldsymbol{v} = 0$, the term containing $\boldsymbol{\omega}$ in Eq. (2) vanishes and the substantial derivative reduces to the partial derivative with respect to the time. In any case, constitutive laws are needed which link $b_{..}$ and $(\delta a_{..}/\delta t)_{\mathrm{irr}}$ with the alignment tensor (and possibly other macroscopic variables). Next, it is indicated how these required relations can be derived.

2. Entropy Production

Within the framework of irreversible thermodynamics, constitutive laws are set up such that the entropy production is non-negative. Point of departure is an equation for the temporal change of the specific entropy s, viz. [1], [4]

$$\frac{\mathrm{d}s}{\mathrm{d}t} = T^{-1}\left(\frac{\mathrm{d}u}{\mathrm{d}t} + P\,\frac{\mathrm{d}\varrho^{-1}}{\mathrm{d}t}\right) - T^{-1}\,\frac{\partial g_{\mathrm{a}}}{\partial a_{\mu\nu}}\,\frac{\mathrm{d}a_{\mu\nu}}{\mathrm{d}t}, \tag{4}$$

where u and ϱ^{-1} are the specific internal energy and volume, respectively, ϱ is the mass density. The quantity g_{a} is the specific Gibbs free energy (chemical potential) associated with the alignment. For fluids of spherical particles or if the orientation of the molecules can be ignored, one has $g_{\mathrm{a}} = 0$. Then (4) reduces to the usual Gibbs relation.

Here, the ansatz

$$g_{\mathrm{a}} = k_{\mathrm{B}}T/m\,[\Sigma + \tfrac{1}{2}\xi_0^2(\nabla_\lambda a_{\mu\nu})(\nabla_\lambda a_{\mu\nu})], \tag{5}$$

with the Landau-type potential [1], [4]

$$\Sigma = \tfrac{1}{2}A\,a_{\mu\nu}a_{\mu\nu} + \tfrac{1}{3}\sqrt{6}\,B\,a_{\mu\nu}a_{\nu\lambda}a_{\lambda\mu} + \tfrac{1}{4}C\,(a_{\mu\nu}a_{\mu\nu})^2 \tag{6}$$

is used. In (5), k_{B} is the Boltzmann constant and m is the mass of a molecule. The dimensionless coefficients A, B, C as well as the "naked" correlation length ξ_0 are functions of the temperature T and the pressure P. The temperature dependence of A is assumed to be given by

$$A = A_0(1 - T^*/T).$$

The characteristic temperature T^* which depends on P is somewhat smaller than the temperature T_{K} where the transition from the isotropic to the nematic phase takes place. The coefficients A_0, B, C are assumed to be practically temperature independent.

In Ref. [1], an expression of the type (5) with (6) and (7) has been used, however without the terms containing the spatial derivatives of $\mathbf{a}$. In Ref. [4], a 4-th order alignment tensor has also been taken into account but again a spatially homogeneous system was considered. Furthermore, in Ref. [1] and [4], the forth order contribution to Σ has been written as

$$\tfrac{1}{4}C_1(a_{\mu\nu}a_{\mu\nu})^2 + \tfrac{1}{4}C_2\,a_{\mu\nu}a_{\nu\lambda}a_{\lambda\varkappa}a_{\varkappa\mu}.$$

However, since $a_{\mu\nu}a_{\nu\lambda}a_{\lambda\varkappa}a_{\varkappa\mu} = \tfrac{1}{2}(a_{\mu\nu}a_{\mu\nu})^2$ for any symmetric traceless tensor $a_{\mu\nu}$, it suffices to use the simpler ansatz (6) with $C = C_1 + \tfrac{1}{2}C_2$.

It should be stressed that (5) is not the most general ansatz as far as the "gradient term" is concerned [3]. Rather, the ansatz was chosen such that it contains the minimal number of phenomenological coefficients associated with the spatial derivatives of the alignment.

Evaluation of $\mathrm{d}g_{\mathrm{a}}/\mathrm{d}t$ with the ansatz (4) and the use of Eq. (2) leads to (ϱ is the mass density of the liquid which is assumed to be constant)

$$\varrho\,\frac{\mathrm{d}s}{\mathrm{d}t} + \nabla_\lambda s_\lambda{}^{\mathrm{a}} = \varrho\left(\frac{\mathrm{d}s}{\mathrm{d}t}\right)_0 - \frac{\varrho}{m}\,k_{\mathrm{B}}\left[\tilde{\Sigma}_{\mu\nu}\left(\frac{\delta a_{\mu\nu}}{\delta t}\right)_{\mathrm{irr}} + b_{\lambda,\,\mu\nu}\nabla_\lambda\tilde{\Sigma}_{\mu\nu}\right] \tag{7}$$

with

$$\tilde{\Sigma}_{\mu\nu} = \Sigma_{\mu\nu} - \xi_0^2\,\Delta a_{\mu\nu}, \tag{8}$$

$$\Sigma_{\mu\nu} = \frac{\partial\Sigma}{\partial a_{\mu\nu}} = A\,a_{\mu\nu} + \sqrt{6}\,B\,\overline{a_{\mu\lambda}a_{\lambda\nu}} + C\,a_{\mu\nu}a_{\lambda\varkappa}a_{\lambda\varkappa}; \tag{9}$$

$(\mathrm{d}s/\mathrm{d}t)_0$ stands for those terms of the change of the entropy which do not involve the alignment. In Eq. (7)

$$s_\lambda{}^{\mathrm{a}} = -\frac{\varrho\,k_{\mathrm{B}}}{m}\left[b_{\lambda,\,\mu\nu}\tilde{\Sigma}_{\mu\nu} - \xi_0^2\,\frac{\mathrm{d}a_{\mu\nu}}{\mathrm{d}t}\,\nabla_\lambda a_{\mu\nu}\right] \tag{10}$$

is the entropy flux density associated with the alignment. The terms in the bracket on the right hand side of Eq. (7) determine the entropy production caused by irreversible changes of the alignment.

Consequences to be inferred from (7) are first considered for $\boldsymbol{v} = 0$, i.e. no flow field.

3. Constitutive Laws, Relaxation Equation

Constitutive laws for $\boldsymbol{v} = 0$ which guarantee that the entropy production associated with the alignment is positive are

$$(\delta a_{\mu\nu}/\delta t)_{\mathrm{irr}} = -\tau_{\mathrm{a}}^{-1}\tilde{\Sigma}_{\mu\nu}, \qquad (11)$$

$$b_{\lambda,\mu\nu} = -D_{\mathrm{a}}\nabla_{\lambda}\tilde{\Sigma}_{\mu\nu}. \qquad (12)$$

The relaxation time τ_{a} and the alignment diffusion coefficient D_{a} have to be positive, i.e., $\tau_{\mathrm{a}} > 0$, $D_{\mathrm{a}} > 0$. In the presence of a viscous flow, additional terms which are linked with the flow alignment occur in (11) cf. Ref. [1] and Section 6. The relation (12) with a single diffusion coefficient again is the simplest ansatz of this type. It is valid provided that the 3 diffusion coefficients for the irreducible parts of rank 1, 2, 3 of the alignment flux tensor $b_{\lambda,\mu\nu}$ are practically equal to each other. For an application where the anisotropy of the diffusion coefficient which is disregarded here is of importance see [5]. It should be mentioned that an additional cross term which links the alignment flux with the heat flux occurs, in general, in (12) if the temperature T is spatially inhomogeneous.

Insertion of (11) and (12) into Eq. (2) yields the nonlinear relaxation equation

$$\partial a_{\mu\nu}/\partial t + \tau_{\mathrm{a}}^{-1}[\tilde{\Sigma}_{\mu\nu} - l_{\mathrm{a}}^2\Delta\tilde{\Sigma}_{\mu\nu}] = 0, \qquad (13)$$

where the length l_{a} is determined by

$$l_{\mathrm{a}}^2 = D_{\mathrm{a}}\tau_{\mathrm{a}}. \qquad (14)$$

Just like ξ_0, l_{a} is expected to be of the order of magnitude of the linear dimension of a molecule.

For $\tilde{\Sigma}_{\mu\nu}$ see (8) and (9).

Some special cases of (13) are discussed next.

4. Isotropic Phase

In the isotropic phase for temperatures not to close to T^*, $\Sigma_{\mu\nu}$ can be approximated by its linear term $A\,a_{\mu\nu}$. Then Eq. (13) reduces to

$$\partial a_{\mu\nu}/\partial t - \tau^{-1}[a_{\mu\nu} - \xi^2\Delta a_{\mu\nu} + \xi'^4\Delta^2 a_{\mu\nu}] = 0, \qquad (15)$$

with the relaxation time

$$\tau = \tau_{\mathrm{a}}A^{-1} = \tau_{\mathrm{a}}A_0^{-1}(1 - T^*/T)^{-1}. \qquad (16)$$

The correlation lengths ξ and ξ' are given by

$$\xi^2 = l_{\mathrm{a}}^2 + A^{-1}\xi_0^2, \qquad (17)$$

$$\xi'^4 = A^{-1}l_{\mathrm{a}}^2\xi_0^2. \qquad (18)$$

Notice that ξ and ξ' contain contributions which stem from the diffusion of the alignment and from the gradient terms in the Gibbs free energy (elastic energy). It should be mentioned however, that terms of the type $(\Delta a..)^2$ in (5) would lead to additional forth order spatial derivative terms in (15).

For temperatures close to T^*, the contribution from l_{a} can be disregarded in (17). Then ξ becomes proportional to $(1 - T^*/T)^{-1/2}$. The correlation length ξ' associated with the 4th order derivative increases slower as T approaches T^* since

$$\xi' \sim (1 - T^*/T)^{-1/4}.$$

From (15) follows, e.g. that the width Γ of the depolrized Rayleigh line (caused by orientational fluctuation) is given by

$$\Gamma = \tau^{-1}[1 + \xi^2 k^2 + \xi'^4 k^4], \qquad (19)$$

where $\boldsymbol{k}$ is the relevant wave vector determined by the scattering geometry. Thus one has

$$\Gamma \sim A + (\xi_0^2 + A\,l_a^2) + O(k^4). \qquad (20)$$

For the intensity I of the scattered radiation one inferres from the free energy (4)

$$I^{-1} \sim A + \xi_0^2 k^2 + O(k^4). \qquad (21)$$

Clearly, the terms involving $\boldsymbol{k}$ in (20) and (21) are different on account of the contributions which stem from the diffusional motion of the molecules. For $A \to 0$, this difference shows up only in the terms of order k^4.

Notice that the width Γ and the intensity I as given by (19, 20, 21) depend on the magnitude of the wave vektor $\boldsymbol{k}$ only. If a more general ansatz for the terms involving the gradient of the alignment tensor [3], [5] is used in the Gibbs free energy (5) and the constitutive relation (12) for the alignment tensor is formulated in full generality [6], the quantities I and Γ also depend on the direction of $\boldsymbol{k}$ and on the polarization vectors of the incident and the scattered light.

5. Nematic Phase, Elasticity Coefficients

For temperatures T smaller than T_{K} which, within the mean field approximation is given by

$$T_{\mathrm{K}} = T^*\left(1 - \frac{2}{9}\frac{B^2}{A_0 C}\right)^{-1} \qquad (22)$$

the thermodynamically stable phase is the nematic phase where the alignment is non-zero [1]. More specifically, the equilibrium alignment is of unaxial form, i.e. one has

$$a_{\mu\nu} = \sqrt{\tfrac{3}{2}}\, a_{\text{eq}}\, \overline{n_\mu n_\nu}\,, \tag{23}$$

where $a_{\text{eq}} = \sqrt{5}\, S = \sqrt{5} \langle P_2(\boldsymbol{n} \cdot \boldsymbol{u}) \rangle$ is a scalar order parameter which is proportional to the Maier-Saupe order parameter S and $\boldsymbol{n}$ is a unit vector (director). Thus for the case where a_{eq} has its equilibrium value determined by

$$\Sigma_{\mu\nu} = 0 \tag{24}$$

but where $\boldsymbol{n}$ is a function of t and $\boldsymbol{r}$, Eq. (13) reduces to

$$\partial/\partial t (n_\mu n_\nu) - \tau_{\text{a}}{}^{-1} \xi_0{}^2 \Delta (1 - l_{\text{a}}{}^2 \Delta)(n_\mu n_\nu) = 0\,. \tag{25}$$

After multiplication of (25) by n_ν and restriction to small fluctuations $\delta\boldsymbol{n}$ about a constant $\boldsymbol{n}^0$ $(\boldsymbol{n}^0 \cdot \delta\boldsymbol{n} \approx 0)$ (25) can be reduced to

$$\partial/\partial t\, \delta n_\mu - \tau_{\text{a}}{}^{-1} \xi_{\text{a}}{}^{-1} \xi_0{}^2 \Delta (1 - l_{\text{a}}{}^2 \Delta)\, \delta n_\mu = 0\,. \tag{26}$$

From (25) and (26) follows qualitatively that $\delta\boldsymbol{n}$ relaxes with an effective relation time

$$\tau_{\text{eff}} \approx \tau_{\text{a}} (L^2/\xi_0{}^2)\, [1 + l_{\text{a}}{}^2 L^{-2}]^{-1} \tag{27}$$

if its spatial variation is characterized by the length L. For a macroscopic length L, the bracket occurring in (27) can be replaced by 1.

Small fluctuations of $\boldsymbol{n}$ about a constant direction $\boldsymbol{n}^0$ are of importance for Rayleigh scattering from the nematic phase. From (26) follows that the line width Γ is given by

$$\Gamma = \tau_{\text{a}}{}^{-1} \xi_0{}^2 k^2 (1 + l_{\text{a}}{}^2 k^2) \tag{28}$$

$\boldsymbol{k}$ is the relevant wave vector.

For the case discussed here, viz. constant magnitude of the alignment, the Gibbs free energy density $G = \varrho g_{\text{a}}$ it follows from (8) with (23) and (24) assumes the form

$$G = \frac{\varrho k_{\text{B}} T}{m} \frac{1}{2} \xi_0{}^2 (\nabla_\lambda a_{\mu\nu})(\nabla_\lambda a_{\mu\nu})\,. \tag{29}$$

For $\boldsymbol{n} = \boldsymbol{n}^0 + \delta\boldsymbol{n}$, $\boldsymbol{n}^0 = \text{const}$, (29) reduces to

$$G = \tfrac{1}{2} K (\nabla_\lambda \delta n_\mu)(\nabla_\lambda \delta n_\mu) \tag{30}$$

with the Frank elasticity coefficient K given by

$$K = \frac{\varrho k_{\text{B}} T}{m} 3\, a_{\text{eq}}^2\, \xi_0{}^2\,. \tag{31}$$

Thus K is related to the length ξ_0 and the magnitude a_{eq} of the alignment.

The property $K \sim a_{\text{eq}}^2$ has been noticed before, e.g. see [3]. It must be stressed, however, that the ansatz (4) was made so simple that all 3 Frank elasticity coefficients become equal. A discussion of the more general case is given in [5].

For a comparison with the notations used in the literature [3] on the dynamical behavior of liquid crystals, it is noticed that (26) can be rewritten as

$$\gamma_1 (\partial/\partial t)\, \delta n_\mu - K \Delta (1 - l_{\text{a}}{}^2 \Delta)\, \delta n_\mu = 0\,, \tag{32}$$

with K given by (31). Leslie coefficient γ_1 is related to the relaxation time τ_{a} by [1]

$$\gamma_{\text{i}} = \tau_{\text{a}} \frac{\varrho k_{\text{B}} T}{m} 3\, a_{\text{eq}}^2\,. \tag{33}$$

Notice that (30) and (33) imply

$$K \gamma_1{}^{-1} = \xi_0{}^2 \tau_{\text{a}}{}^{-1}\,. \tag{34}$$

This quantity has the dimension of a diffusion coefficient which is sometimes [3] referred to as orientational diffusion coefficient.

6. Flow Alignment, Friction Pressure Tensor

In the presence of a viscous flow with flow velocity $\boldsymbol{v} = \boldsymbol{v}(\boldsymbol{r})$, the relaxation equation (2) contains additional terms on the left hand side as already indicated in Section 1. Furthermore, the entropy production $(\mathrm{d}s/\mathrm{d}t)_0$ involves a term proportional to $\overline{p_{\mu\nu}}\, \overline{\nabla_\mu v_\nu}$ where $\overline{p_{\mu\nu}}$ is the symmetric traceless part of the friction pressure tensor. The constitutive laws for the 2nd rank tensors $(\delta a_{\mu\nu}/\delta t)_{\text{irr}}$ and $\overline{p_{\mu\nu}}$, in general, contain cross terms associated with flow alignment and its reciprocal phenomenon. In analogy to the equations stated in Ref. [1] for a spatially homogeneous alignment, one now obtains for the spatially inhomogeneous case

$$\frac{\mathrm{d}}{\mathrm{d}t} a_{\mu\nu} - 2\, \overline{\varepsilon_{\mu\lambda\varkappa}\, \omega_\lambda\, a_{\varkappa\nu}} + \tau_{\text{a}}{}^{-1} [(1 - l_{\text{a}}{}^2 \Delta)\, \tilde{\Sigma}_{\mu\nu} + \sqrt{2}\, \tau_{\text{ap}}\, \overline{\nabla_\mu v_\nu}] = 0\,, \tag{35}$$

$$\overline{p_{\mu\nu}} = -\frac{\varrho k_{\text{B}} T}{m} \Big[2\, \tau_{\text{p}}\, \overline{\nabla_\mu v_\nu} + \sqrt{2}\, \tau_{\text{pa}} \Big(\frac{\mathrm{d} a_{\mu\nu}}{\mathrm{d}t} - 2\, \overline{\varepsilon_{\mu\lambda\varkappa}\, \omega_\lambda\, a_{\varkappa\nu}} + \nabla_\lambda b_{\lambda,\mu\nu} \Big) \Big]\,, \tag{36}$$

with

$$\frac{d}{\mathrm{d}t} = \frac{\partial}{\partial t} + v_\lambda \nabla_\lambda\,, \quad \boldsymbol{\omega} = \tfrac{1}{2} \boldsymbol{\nabla} \times \boldsymbol{v}\,. \tag{37}$$

The "nondiagonal" relaxation times obey the Onsager symmetry relation $\tau_{\mathrm{ap}} = \tau_{\mathrm{pa}}$ and one has $\tau_{\mathrm{ap}}^2 < \tau_{\mathrm{a}} \tau_{\mathrm{p}}$.

Again, just as for the pure relaxation case, the equation (35) can be linearized about its zero and nonzero equilibrium value for the alignment in the isotropic and nematic phases, respectively, provided that the temperature T is not to close to the transition temperature T_{K}.

Thus, analogous to (26) and (32) the equation governing the director $\boldsymbol{n}$ in the nematic phase which follows from (35) can be written as

$$\boldsymbol{n} \times \left[\gamma_1 \frac{\mathrm{d}\boldsymbol{n}}{\mathrm{d}t} - K \Delta \boldsymbol{n} + \gamma_2 \overline{\nabla \boldsymbol{v}} \cdot \boldsymbol{n}\right] = 0, \quad (38)$$

with the 2nd Leslie coefficient γ_2 given by [1]

$$\gamma_2 = \frac{\varrho k_{\mathrm{B}} T}{m} 2\sqrt{3}\, a_{\mathrm{eq}} \tau_{\mathrm{ap}}. \quad (39)$$

In (38), terms involving Δ^2 have been disregarded.

Concluding Remarks

The Eq. (38) is a well-known relation [3] which is of importance for many applications [7], [8] of nematic liquid crystals. It is the advantage of the present approach that firstly, it is derived from Eq. (35) which is valid both in the isotropic and nematic phases. Secondly, the phenomenological coefficients K, γ_1, γ_2 are expressed in terms of the coefficients ξ_0, τ_{a}, τ_{ap} (which are meaningful in both phases) and the equilibrium alignment a_{eq}. For a discussion of the dependence of γ_1, γ_2 on a_{eq} see also [9], [10]. It should be mentioned that a continuity of the "naked" coefficients τ_{a} and τ_{ap} at the isotropic-nematic phase transition temperature has been noticed before [11], see also [10].

The previously presented applications of Eq. (35) with spatially homogeneous alignment to a study of the pre- and post-transitional behavior of the flow alignment of a liquid crystal [12] as well as to an analysis of the non-newtonian viscosity [13] and the viscoelasticity [14] of a molecular liquid can be extended to the case where the alignment is spatially inhomogeneous. Then, of course, boundary conditions are needed for the alignment tensor. A method for the derivation of systematic bondary conditions has been invented by Waldmann [15]. It makes use of the entropy flux which in the present case is given by Equation (10). The boundary conditions are linear relations, e.g. between $b_{\lambda,\mu\nu}$ and $\Sigma_{\mu\nu}$ which ensure the entropy production at the interface between the liquid crystal and a solid wall is positive definite. Consequences of these boundary conditions then have to be studied for specific geometries and experimental situations.

Various applications to transport processes and non-equilibrium alignment phenomena in gases have been worked out by Waldmann and Vestner [15], [16]. These methods can be adapted to the corresponding phenomena in liquid crystals.

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