

# Incompressibility Conditions in Liquid Crystals

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## Abstract

We discuss the implications of the incompressibility approximation on the number of relevant transport parameters, like viscosities, flow alignment coefficients, and rotational viscosities in uniaxial and biaxial nematic liquid crystals. A comparison between the hydrodynamic and the Leslie-Ericksen approach is given. Agreement is found, if in the latter description a redefinition of the pressure is assumed. For systems with positional order, like smectic and columnar liquid crystals and crystals, we show that, generally, incompressibility does not imply that the displacement field is source-free.

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## 1 Introduction and Results

The dynamic description of uniaxial nematic liquid crystals has been pioneered by Ericksen [1–3] and Leslie [4, 5]. Starting from a continuum-mechanics description of conservation laws a very general set of additional constitutive equations is given for a wide range of different materials. With further specifications and assumptions (including incompressibility) these equations are then adjusted for the case of uniaxial nematics. They have been proven to be rather successful in describing experiments. Treatments using the alignment (or anisotropy or order parameter) tensor instead of the director followed [6]. In the same spirit approaches using Poisson brackets to derive the reversible [7] and the dissipative part [8] of the dynamics have been pursued. A Leslie-Ericksen type theory for biaxial nematics can be found in [9]. For nematic polymers similar equations have been derived [10] starting from a microscopic model. There are no Leslie-Ericksen type theories describing the elastic degrees of freedom in smectic, columnar or crystal systems.

Another approach has been introduced in [11], where the notion of spontaneously broken continuous symmetries is used. Since every such broken symmetry gives rise

to a hydrodynamic mode (in the absence of unscreened long-ranged forces), the exact number and the correct nature of the relevant variables is obtained. Thermodynamics and symmetry considerations then lead to the dynamic equations without any additional assumptions. This method (cf. ref. [12] for a detailed exposition) is applicable to systems with spontaneously broken continuous symmetries of any kind (e.g. biaxial nematics [13, 14]) including strong external fields [15] and can be generalized to systems with slow non-hydrodynamic variables (like nematic polymers [16]). These theories describe generally the compressible case and the incompressibility approximation can be implemented explicitly, in order to compare with the Leslie-Ericksen approach. Agreement, at least with respect to the number of material parameters involved, has been found [17] for uniaxial nematics rather early. Here we give a detailed discussion how incompressibility has to be established in uniaxial and biaxial systems as well as in systems with elastic degrees of freedom.

We start with the well-known example of simple liquids, where incompressibility is easy to implement. We carry over this procedure straightforwardly to uniaxial nematics. Comparison with the Leslie-Ericksen equations shows that agreement is obtained only, if in the latter approach the pressure is identified not with the usual thermostatic pressure, but with a redefined one that contains contributions from the actual flow field. A similar discussion is provided for the biaxial case. Here, explicit formulas for the material tensors (like viscosity, flow alignment, and rotational viscosity tensor) are given, not only for orthorhombic symmetry, but also for mono- and triclinic, as well as tetragonal, hexagonal and cubic symmetries, most of which have never been shown before. Again, comparison with appropriate Leslie-Ericksen type theories (when available) shows that agreement implies the redefinition of the pressure in the latter case, while without such a pressure redefinition the number of viscosities is considerably larger in the hydrodynamic case. Quite generally, the degree of simplification that is reached by assuming incompressibility diminishes drastically for the more complicated systems (of rather low symmetry).

In the last section we deal with elastic degree(s) of freedom in smectic, discotic and crystal systems, which describe layer compression (or dilation), lattice compression and in-plane shear of the column lattice, and ordinary elasticity, respectively. In the smectic and columnar phases incompressibility does neither affect the displacement field, which describes elasticity, nor its dynamic equation. Thus, the assumption of constant layer spacing in smectics is an additional approximation, which is completely unrelated and independent of incompressibility, and leads to additional constraints on the flow field well beyond the incompressibility approximation. In crystals incompressibility implies the divergence of the displacement field to be zero (source-free) only in the isotropic case (disordered solids), while for all crystal symmetries a special compatibility condition involving the displacement field and its time derivative is obtained. Only if, additionally, vacancy diffusion is neglected, incompressibility requires a source-free displacement field.

## 2 Simple Fluids

As a pedagogical example we start with a discussion of incompressibility in simple liquids. Omitting the thermal degree of freedom for simplicity, isotropic Newtonian fluids are described by the dynamic equations for the mass density  $\rho$  and the velocity  $v_i$

$$\dot{\rho} + \nabla_i \rho v_i = 0 \quad (1)$$

$$\rho(\dot{v}_i + v_j \nabla_j v_i) + \nabla_i p + \nabla_j \sigma_{ij} = 0 \quad (2)$$

which represent mass and momentum conservation. A dot means partial derivation with respect to time and  $\nabla_i$  is the spatial gradient. The thermodynamic pressure  $p$  is defined as  $p = -dF/dV$  with  $V$  the volume and  $F$  the total energy of the system. In the Newtonian limit the stress tensor  $\sigma_{ij}$  reads

$$\sigma_{ij} = -2\nu(A_{ij} - \frac{1}{3}\delta_{ij}A_{kk}) - \zeta\delta_{ij}A_{kk} \quad (3)$$

with  $2A_{ij} = \nabla_i v_j + \nabla_j v_i$ . There are 2 transport parameters,  $\nu$  the shear and  $\zeta$  the compressional viscosity. Changes of the pressure are related to density changes by the (linear) static relation

$$\delta p = c_s^2 \delta \rho \quad (4)$$

with  $c_s$  the sound velocity. For simplicity the material parameters  $\nu$ ,  $\zeta$  and  $c_s$  will be treated as constants.

If we linearize around a state of constant density ( $\rho_0$ ) and zero velocity, the bulk dynamics eqs.(1-3) can be decomposed

$$\dot{\rho} + \rho_0 \operatorname{div} \mathbf{v} = 0 \quad (5)$$

$$\rho_0 \operatorname{div} \dot{\mathbf{v}} + \Delta p - (\zeta + \frac{4}{3}\nu)\Delta \operatorname{div} \mathbf{v} = 0 \quad (6)$$

$$\rho_0 \operatorname{curl} \dot{\mathbf{v}} - \nu \Delta \operatorname{curl} \mathbf{v} = 0 \quad (7)$$

into a longitudinal ( $\rho$  and  $\operatorname{div} \mathbf{v}$ ) and a transverse part ( $\operatorname{curl} \mathbf{v}$ ) describing sound waves and vorticity diffusion, respectively ( $\Delta = \nabla^2$  is the Laplacian). It should be noted that this splitting of the dynamics into two separate parts is peculiar for simple, isotropic liquids and does generally not hold for more complicated systems like liquid crystals.

It is now easy to see how the incompressibility condition can be invoked: The density remains constant for all times, if  $\dot{\rho} = 0$ , which immediately leads to the familiar condition  $\operatorname{div} \mathbf{v} = 0$ . This is compatible with eq.(6) only if

$$\Delta p = 0 \quad (8)$$

This condition replaces the static relation (4), since changes of  $\rho$  are zero, i.e.  $\rho$  is no longer a variable. Of course, the pressure can vary in space and time even under the assumption of incompressibility (provided (8) holds). This fact is reconciled with eq.(4) by the formal requirement  $c_0 \rightarrow \infty$ , because then  $c_0^2 \delta \rho$  is undefined, eq. (4) is void, and the pressure follows from (8). This is the reason why incompressibility is assumed to be a good approximation for flows with velocities well below the sound velocity.

Since the incompressibility condition only affects the longitudinal part of the dynamics, the remaining transverse dynamics (7) is unchanged. It contains only the shear viscosity  $\nu$  as material parameter. The compressional viscosity  $\zeta$  has dropped out automatically and it does not matter whether it is small or large compared to  $\nu$ . The true approximation that is related to 'incompressibility' is  $c_0 \rightarrow \infty$ . In addition, the boundary conditions at free surfaces also do not contain  $\zeta$ . There, normal stresses  $p + \hat{N}_i \hat{N}_j \sigma_{ij}$  are balanced by surface tension while shear stresses  $\hat{P}_i \hat{N}_j \sigma_{ij}$  are zero ( $\hat{N}_i$  and  $\hat{P}_i$  are unit vectors normal and parallel to the surface, respectively).

This picture is basically unchanged also in the nonlinear case. Assuming the density to be constant in time and space we get  $\operatorname{div} \mathbf{v} = 0$ . The compatibility condition for the pressure (8) is more complicated in the nonlinear case

$$\Delta p = -\rho \nabla_i \nabla_j v_i v_j \quad (9)$$

but again  $\zeta$  drops out and  $c_0 \rightarrow \infty$  is the relevant approximation.

### 3 Compressible Uniaxial Nematics

Uniaxial nematic liquid crystals differ from simple liquids not only by their lower symmetry due to the preferred direction (denoted by the director  $\hat{\mathbf{n}}$ ), but also by additional hydrodynamic degrees of freedom, rotations of  $\mathbf{n}$ . Their full hydrodynamic equations are well known [11] and can be written as (for more details and a derivation of the equations see [12])

$$\dot{n}_i + v_j \nabla_j n_i - \frac{1}{2} \lambda_{ijk} \nabla_j v_k + \frac{1}{\gamma_1} \delta_{ik}^\perp h_k = 0 \quad (10)$$

where the flow alignment tensor

$$\lambda_{ijk} = (\lambda - 1) \delta_{ij}^\perp n_k + (\lambda + 1) \delta_{ik}^\perp n_j \quad (11)$$

contains the director reorientations due to rotational flow (antisymmetric part) and due to elongational flow (symmetric part with the reactive material parameter  $\lambda$  that controls flow alignment of the director e.g. in shear flows). The transverse Kronecker tensor  $\delta_{ij}^\perp = \delta_{ij} - n_i n_j$  guarantees  $\mathbf{n}^2 = 1$  for all times. The dissipative material parameter  $\gamma_1$  (sometimes called orientational viscosity) governs the orientation diffusion (or relaxation if an external field is present) of the director, since

$$h_i = \frac{\delta}{\delta n_i} F^{(n)} \quad \text{with} \quad 2F^{(n)} = \int dV (K_{ijkl} (\nabla_j n_i) (\nabla_l n_k) - \epsilon_a (\mathbf{n} \cdot \mathbf{E})^2) \quad (12)$$

where the director-dependent part of the total energy  $F^{(n)}$  contains the Frank orientational elastic energy [17] (with 3 coefficients  $K_{1,2,3}$ ) as well as the dielectric anisotropy energy ( $\sim \epsilon_a$ ) due to an external electric field  $\mathbf{E}$ , which we will assume to be constant in the following.

The form of the continuity (1) and the Navier-Stokes equation (2) remains unchanged, however the stress tensor is more complicated

$$\sigma_{ij} = -\nu_{ijkl} A_{kl} - \frac{1}{2} \lambda_{kji} h_k + K_{qjkl} (\nabla_l n_k) (\nabla_i n_q) \quad (13)$$

since it contains not only viscous effects ( $\nu_{ijkl}$ ) but also 'back flow' (changes in the flow due to director reorientation) governed by the flow alignment tensor; in addition there is the nonlinear so-called Ericksen stress. Note that the flow alignment and the back flow effect come with the same material parameter ensuring that they cancel each other in the entropy production, which is required by their (time) reversible character. The viscosity tensor reflects the uniaxial symmetry of nematics and reads in the notation of [19]

$$\begin{aligned} \nu_{ijkl} = & \nu_2 (\delta_{jl} \delta_{ik} + \delta_{il} \delta_{jk}) + 2(\nu_1 + \nu_2 - 2\nu_3) n_i n_j n_k n_l + (\nu_5 - \nu_4 + \nu_2) (\delta_{ij} n_k n_l + \delta_{kl} n_i n_j) \\ & + (\nu_4 - \nu_2) \delta_{ij} \delta_{kl} + (\nu_3 - \nu_2) (n_j n_l \delta_{ik} + n_j n_k \delta_{il} + n_i n_k \delta_{jl} + n_i n_l \delta_{jk}) \end{aligned} \quad (14)$$

containing 5 independent viscosity parameters. Pressure variations are also slightly more complicated in nematics compared to simple fluids and given by

$$\nabla_i p = \rho \nabla_i \mu + \sigma \nabla_i T + \rho v_j \nabla_i v_j - h_j \nabla_i n_j \quad (15)$$

relating the pressure to the chemical potential  $\mu$ , to the temperature  $T$  (thermodynamically conjugate to the entropy density  $\sigma$ ), to flow (in a nonlinear fashion) and to the director degrees of freedom.

For the thermal degree of freedom we need a dynamical equation (for other possible macroscopic degrees of freedom, like concentration in lyotropic systems, order parameter fluctuations in polymeric systems and charge density in conducting systems see [12]), e.g. in the form of an entropy balance equation

$$\dot{\sigma} + \nabla_i(v_i\sigma) - \nabla_j(\kappa_{ij}\nabla_i T) = \frac{R}{T} \quad (16)$$

where the source term  $R$  is the entropy production, which is zero for reversible processes (where the entropy is conserved) and positive for dissipative ones (second law of thermodynamics). In our case the dissipative processes are viscosity, director diffusion (or relaxation in the presence of an external electric field) and heat conduction, the latter expressed in (16) by the heat conduction tensor  $\kappa_{ij} = \kappa_{\parallel}n_in_j + \kappa_{\perp}\delta_{ij}^{\perp}$ . This gives rise to the entropy production

$$2R = \gamma_1^{-1}\delta_{ij}^{\perp}h_i h_j + \nu_{ijkl}A_{ij}A_{kl} + \kappa_{ij}(\nabla_i T)(\nabla_j T) \quad (17)$$

which is bilinear in the thermodynamic forces (and thus also in the dynamic variables) and contains 8 dissipative material parameters. For the conditions on these parameters to guarantee positivity of  $R$  we refer to [12]. Using the entropy production  $R$  as potential to derive the dissipative parts of the currents (and  $R = 0$  for the reversible ones) automatically guarantees all possible Onsager relations. Together with the flow alignment parameter  $\lambda$  this makes 9 transport parameters in total, one of which ( $\lambda$ ) is reactive (and not restricted in its value by thermodynamics).

To close the system of hydrodynamic equations we have to express the conjugate variables  $T$  and  $\mu$  by the dynamic ones ( $\rho$  and  $\sigma$ ); since all quantities are scalars these relations are identical to those in simple fluids

$$\delta T = \frac{T}{C_V} \delta\sigma + \frac{1}{\rho\alpha_s} \delta\rho \quad (18)$$

$$\delta\mu = \frac{1}{\rho^2\kappa_s} \delta\rho + \frac{1}{\rho\alpha_s} \delta\sigma \quad (19)$$

and follow from a free energy density  $2f_0 = TC_V^{-1}(\delta\sigma)^2 + \rho^{-2}\kappa_s^{-1}(\delta\rho)^2 + 2\rho^{-1}\alpha_s^{-1}(\delta\rho)(\delta\sigma)$  containing 3 static susceptibilities, the adiabatic compressibility  $\kappa_s$ , the specific heat at constant density  $C_V$ , and the adiabatic volume expansion coefficient  $\alpha_s$ . Together with the 3 Frank orientational elastic constants this makes 6 static susceptibilities in total (in the absence of external fields). Using the Gibbs-Duhem equation (15) the pressure can be expressed by the variables and the system of dynamic equations is closed. Solving for sound waves the sound velocity is found to be  $\rho c_0^2 = 1/\kappa_s + 2\sigma/\alpha_s + \sigma^2 T/C_V \approx 1/\kappa_s$ .

## 4 Incompressible Uniaxial Nematics

Incompressibility means that the density is constant in time and space. Thus,  $\rho$  is eliminated as hydrodynamic variable and does not occur in the free energy density  $f =$

$f(\{\text{variables}\})$  anymore. Therefore, the chemical potential  $\mu \equiv \partial f / \partial \rho$  is not defined and eq.(18) is replaced by

$$\delta T = \frac{T}{C_V} \delta \sigma \quad (20)$$

or  $2f_0 = TC_V^{-1}(\delta\sigma)^2$ , which can be reconciled with the compressible case by the formal limit of zero compressibility  $\kappa_s \rightarrow 0$  and zero volume expansion  $\alpha_s \rightarrow 0$ . Since there are no volume changes, the Gibbs-Duhem relation (15) does not exist.

Of course, mass conservation still holds and eq.(1) has to be fulfilled, which requires  $\text{div} \mathbf{v} = 0$  everywhere and for all times. This in turn is guaranteed by the conditions

$$\Delta p = -\rho \nabla_i \nabla_j v_i v_j + \nabla_i \nabla_j \nu_{ijkl} A_{kl} + \nabla_i \nabla_j \frac{1}{2} \lambda_{kji} h_k - \nabla_i \nabla_j K_{qjkl} (\nabla_l n_k) (\nabla_i n_q) \quad (21)$$

or linearized

$$\begin{aligned} \Delta p = & \lambda n_k \nabla_k \text{div} \mathbf{h} + (2\nu_3 - \nu_2 - \nu_4 + \nu_5) n_k n_j \nabla_j \Delta v_k \\ & + 2(\nu_1 + \nu_2 - 2\nu_3) n_i n_j n_k n_l \nabla_i \nabla_j \nabla_k v_l \end{aligned} \quad (22)$$

which are the nematic analogue to (8) and (9).

The momentum balance equation (2) is somewhat simplified by the incompressibility condition  $\text{div} \mathbf{v} = 0$  and reads in linearized form

$$\begin{aligned} \rho \dot{v}_i + \nabla_i p - \frac{1}{2} \nabla_j \lambda_{kji} h_k - \nu_2 \Delta v_i - 2(\nu_1 + \nu_2 - 2\nu_3) n_i n_j n_k n_l \nabla_j \nabla_k v_l \\ - (\nu_5 - \nu_4 + \nu_2) n_k n_l \nabla_i \nabla_k v_l - (\nu_3 - \nu_2) (n_k n_i \Delta v_k + n_j n_l \nabla_k \nabla_l v_i) = 0 \end{aligned} \quad (23)$$

while the form of the director rotation equation (10) is unchanged. The linearized boundary conditions for free boundaries can be written as

$$\begin{aligned} \hat{P}_i \hat{N}_j \left( \nu_2 (\nabla_i v_j + \nabla_j v_i) + (\nu_3 - \nu_2) (n_j n_l \nabla_i v_l + n_j n_l \nabla_l v_i + n_l n_i \nabla_j v_l + n_l n_i \nabla_l v_j) \right. \\ \left. + \frac{1}{2} \lambda_{kji} h_k \right) = 0 \end{aligned} \quad (24)$$

and

$$\begin{aligned} \hat{N}_i \hat{N}_j \left( \delta_{ij} p - 2\nu_2 \nabla_i v_j - 2(\nu_1 + \nu_2 - 2\nu_3) n_i n_j n_k n_l \nabla_k v_l - \delta_{ij} (\nu_5 - \nu_4 + \nu_2) n_k n_l \nabla_k v_l \right. \\ \left. - (\nu_3 - \nu_2) (n_j n_l \nabla_i v_l + n_j n_l \nabla_l v_i + n_l n_i \nabla_j v_l + n_l n_i \nabla_l v_j) + \frac{1}{2} \lambda_{kji} h_k \right) = C \end{aligned} \quad (25)$$

where  $\hat{N}_i$  and  $\hat{P}_i$  are unit vectors, normal and parallel to the surface, respectively, and  $C$  is the curvature stress due to surface tension. Eqs.(21-25) still contain 4 linear combinations out of the 5 viscosities of uniaxial nematics. This number can be further reduced by redefining the pressure

$$p' \equiv p - (\nu_5 - \nu_4 + \nu_2) n_k n_l \nabla_k v_l \quad (26)$$

eliminating the combination  $\nu_5 - \nu_4 + \nu_2$  from the system of dynamic equations. Only 3 combinations of viscosities, which involve  $\nu_{1,2,3}$  only, are left. Together with  $\gamma_1$  from the director equation there are 5 transport parameters (one of which ( $\lambda$ ) is reactive) and 4 static susceptibilities ( $K_{1,2,3}$  and  $C_V$ ) remaining. Of course, this reduction to 3 relevant viscosity combinations is obtained for the prize that  $p'$  has no simple physical

meaning. It could be argued that in the true incompressible limit pressure is not defined anyhow and cannot be measured statically. In that case  $p$  or  $p'$  are dummy variables that can be eliminated completely from the set of equations. However, incompressibility is an approximation, often used to simplify the description of flows, and appropriate for velocities well below the sound velocity and for situations, where the thermal expansion is negligible. In most situations where this approximation is used, the pressure  $p$  can still be interpreted and measured as the hydrostatic pressure. Then, of course, the difference  $p - p'$  matters.

In isotropic liquids such a redefinition of the pressure is neither appropriate nor necessary, since there the dynamics comes in two separate parts and the pressure does not occur in that part, which is relevant for the incompressible case. Such a separation into a longitudinal part ( $p$  and  $div\mathbf{v}$ ) and a transverse part ( $curl\mathbf{v}$ ) is not possible in liquid crystal phases nor in anisotropic crystals [18].

There have been different procedures in the literature to reduce the full compressible dynamics to the incompressible case. A common trick is to give special values to some of the viscosities, such that, e.g. no  $div\mathbf{v}$  terms are left in the stress tensor (and thus in the boundary conditions). This leads to [17, 19]  $\nu_2 = \nu_4$  and  $\nu_5 = 0$ . These are purely formal relations, which generally have no correspondence to reality (for isotropic fluids this procedure would give  $\zeta = 2\nu/3$ , which again is far off the experimental values). Worse, they do not eliminate  $div\mathbf{v}$  from the dynamics, i.e. from  $\nabla_j\sigma_{ij}$ . For that case different conditions,  $\nu_4 = 0$  and  $\nu_3 + \nu_5 = 0$  are necessary (for isotropic fluids the corresponding relation would be  $\zeta = -\nu/3$ , which would violate the second law of thermodynamics). But these conditions do not guarantee  $div\mathbf{v} = 0$  for all times. To get this  $\nu_5 = \nu_4 + \nu_1$ ,  $\nu_1 + \nu_2 = \nu_3$ , and even  $\lambda = 0$  have been proposed [20], in which case eq.(21) reduces to  $\Delta p = 0$ . Obviously neither of these attempts can completely eliminate  $div\mathbf{v}$  from the whole set of equations and the proper procedure is that described above.

Historically the first to derive dynamical equations for incompressible uniaxial nematics were Ericksen [1–3] and Leslie [4, 5]. From a rather large set of dynamic equations, which contains several non-hydrodynamic variables, they distill equations that can be compared with the hydrodynamic ones. The dynamic equation for the director is thereby formulated as a balance of torques acting on the director. Their equations are compatible with (10) and (23), if one interprets their pressure as the redefined pressure (26). In that case the 5 'viscosities'  $\alpha_{1-5}$  (a sixth one is dependent due to an Onsager relation  $\alpha_6 = \alpha_5 + \alpha_3 + \alpha_2$ ) introduced in their theory can be related to the transport coefficients used here by [12, 17]

$$\begin{aligned}
\alpha_1 &= 2(\nu_1 + \nu_2 - 2\nu_3) - \gamma_1\lambda^2 \\
2\alpha_2 &= -\gamma_1(1 + \lambda) \\
2\alpha_3 &= \gamma_1(1 - \lambda) \\
\alpha_4 &= 2\nu_2 \\
2\alpha_5 &= 4(\nu_3 - \nu_2) + \gamma_1\lambda(\lambda + 1)
\end{aligned} \tag{27}$$

which in turn shows that the reactive parameter  $\lambda = (\alpha_2 + \alpha_3)/(\alpha_2 - \alpha_3)$  is expressed as the ratio of dissipative ones.

## 5 Biaxial Nematics

Biaxial nematic liquid crystals are characterized by the existence of two different directors  $\mathbf{n}$  and  $\mathbf{m}$  (defining a third one,  $\mathbf{p} \sim \mathbf{n} \times \mathbf{m}$ ). A nonlinear hydrodynamic description has been given in (the second part of) [13] and in [14], while a Leslie-Ericksen type treatment can be found in [9]. If the two directors are orthogonal (oblique), the phase is of orthorhombic  $D_{2h}$  (monoclinic  $C_{2h}$ ) symmetry. In the case that two (all three) of the directors are equivalent, i.e. if there is a  $\mathbf{n} \leftrightarrow \mathbf{m}$  ( $\mathbf{n} \leftrightarrow \mathbf{m} \leftrightarrow \mathbf{p} \leftrightarrow \mathbf{n}$ ) symmetry, the symmetry is raised to tetragonal  $D_{4h}$  (cubic  $O_h$ ). If there are 3 different directors, neither of which is orthogonal to any of the others, the lowest symmetry, triclinic  $C_i$  is obtained, where only a center of inversion exists.

Table 1: This table shows for different systems the number of viscosities in the compressible ( $\nu_{comp}$ ) and in the incompressible case, without ( $\nu_{inc}$ ) and with ( $\nu_p$ ) redefining the pressure. In addition the number of reactive flow alignment parameters in the compressible ( $\lambda_{comp}$ ) and the incompressible case ( $\lambda_{inc}$ ), as well as the director orientational viscosities ( $\gamma$ ) is listed. The columns  $\nu_p$ ,  $\lambda_{inc}$ , and  $\gamma$  add up to the number of Leslie-Ericksen parameters ( $LE$ ).

symmetry	$\nu_{comp}$	$\nu_{inc}$	$\nu_p$	$\gamma$	$\lambda_{comp}$	$\lambda_{inc}$	$LE$
isotropic	2	1	1	–	–	–	–
uniaxial/hexagonal	5	4	3	1	1	1	5
biaxial orthorhombic	9	8	6	3	3	3	12
biaxial monoclinic	13	12	9	4	8	7	20
biaxial triclinic	21	20	15	6	18	15	(36)
biaxial tetragonal	6	5	4	2	1	1	(7)
biaxial cubic	3	2	2	1	0	0	(3)

In the compressible case the viscosity tensor has the same symmetry properties, and thus the same form as, the elastic tensor. The number of independent viscosity coefficients can therefore be read off textbooks [21] and are found to be 21, 13, 9, 6, and 3 for triclinic, monoclinic, orthorhombic, tetragonal ( $D_{4h}$ ), and cubic symmetry, respectively (Table (1)). For the most important orthorhombic case the viscosity tensor has the form [13] ( $\mathbf{p} = \mathbf{n} \times \mathbf{m}$ )

$$\begin{aligned}
\nu_{ijkl}^{(ortho)} = & \nu_1 m_i m_j m_k m_l + \nu_2 n_i n_j n_k n_l + \nu_3 p_i p_j p_k p_l + \nu_4 (m_k m_l n_i n_j + m_i m_j n_k n_l) \\
& + \nu_5 (m_k m_l p_i p_j + m_i m_j p_k p_l) + \nu_6 (n_k n_l p_i p_j + n_i n_j p_k p_l) \\
& + \nu_7 (m_j m_l n_i n_k + m_j m_k n_i n_l + m_i m_k n_j n_l + m_i m_l n_j n_k) \\
& + \nu_8 (m_j m_l p_i p_k + m_j m_k p_i p_j + m_i m_k p_j p_l + m_i m_l p_j p_k) \\
& + \nu_9 (n_j n_l p_i p_k + n_j n_k p_i p_l + n_i n_k p_j p_l + n_i n_l p_j p_k)
\end{aligned} \tag{28}$$



For the mono- and triclinic case additional terms are present

$$\begin{aligned}
\nu_{ijkl}^{(mono)} &= \nu_{ijkl}^{(ortho)} + \nu_{10}(m_i m_j m_k n_l + m_i m_j m_l n_k + m_k m_l m_i n_j + m_k m_l m_j n_i) \\
&+ \nu_{11}(n_i n_j n_k m_l + n_i n_j n_l m_k + n_k n_l n_i m_j + n_k n_l n_j m_i) \\
&+ \nu_{12}(p_i p_j m_k n_l + p_i p_j m_l n_k + p_k p_l m_i n_j + p_k p_l m_j n_i) \\
&+ \nu_{13}(p_i p_k m_j n_l + p_j p_k m_i n_l + p_i p_l m_j n_k + p_j p_l m_i n_k \\
&\quad + p_i p_k m_l n_j + p_l p_i m_k n_j + p_k p_j m_l n_i + p_j p_l m_k n_i)
\end{aligned} \tag{29}$$

and

$$\begin{aligned}
\nu_{ijkl}^{(tric)} &= \nu_{ijkl}^{(mono)} + \nu_{14}(m_i m_j m_k p_l + m_i m_j m_l p_k + m_k m_l m_i p_j + m_k m_l m_j p_i) \\
&+ \nu_{15}(n_i n_j n_k p_l + n_i n_j n_l p_k + n_k n_l n_i p_j + n_k n_l n_j p_i) \\
&+ \nu_{16}(p_i p_j p_k n_l + p_i p_j p_l n_k + p_k p_l p_i n_j + p_k p_l p_j n_i) \\
&+ \nu_{17}(p_i p_j p_k m_l + p_i p_j p_l m_k + p_k p_l p_i m_j + p_k p_l p_j m_i) \\
&+ \nu_{18}(m_i m_j p_k n_l + m_i m_j p_l n_k + m_k m_l p_i n_j + m_k m_l p_j n_i) \\
&+ \nu_{19}(n_i n_j p_k m_l + n_i n_j p_l m_k + n_k n_l p_i m_j + n_k n_l p_j m_i) \\
&+ \nu_{20}(m_i m_k p_j n_l + m_j m_k p_i n_l + m_i m_l p_j n_k + m_j m_l p_i n_k \\
&\quad + m_k m_i p_l n_j + m_l m_i p_k n_j + m_k m_j p_l n_i + m_j m_l p_k n_i) \\
&+ \nu_{21}(n_i n_k p_j m_l + n_j n_k p_i m_l + n_i n_l p_j m_k + n_j n_l p_i m_k \\
&\quad + n_i n_k p_l m_j + n_l n_i p_k m_j + n_k n_j p_l m_i + n_j n_l p_k m_i)
\end{aligned} \tag{30}$$

where in (29)  $\mathbf{p} \equiv (\mathbf{n} \times \mathbf{m})(1 - (\mathbf{n} \cdot \mathbf{m})^2)^{-1/2}$ , while in (30)  $\mathbf{p}$  has to be an independent additional director.

For the tetragonal and cubic case some of the viscosities in (28) have to be equal, i.e.  $\nu_1 = \nu_2$ ,  $\nu_5 = \nu_6$ ,  $\nu_8 = \nu_9$  and  $\nu_1 = \nu_2 = \nu_3$ ,  $\nu_4 = \nu_5 = \nu_6$ ,  $\nu_7 = \nu_8 = \nu_9$ , respectively.

In the incompressible case the number of relevant viscosities is smaller. It is easy to see that there is exactly one (and only one) compressional viscosity irrespective of the symmetry of the phase: connecting two scalar quantities, the pressure  $p$  with  $\text{div} \mathbf{v}$ , it has to be a scalar, too. Thus, strictly speaking, the number of viscosities in the incompressible case is lowered just by one compared to the compressible case (Table (1)). In (28) a linear combination of the first 6 terms ( $T_1 + T_2 + T_3 + T_4 + T_5 + T_6$ ) gives the compressional contribution  $\sim \delta_{ij} \delta_{kl}$ , which, in the incompressible limit, drops out automatically from the free boundary conditions, from the dynamics (including  $\nu_{ijkl} \nabla_j A_{kl}$ ), and from the compatibility condition for  $\Delta p$  (containing  $\nu_{ijkl} \nabla_i \nabla_j A_{kl}$ ).

There are terms in the viscosity tensor that are partially related to  $\text{div} \mathbf{v}$ . They have the form  $\delta_{ij}(\bar{\nu}_{kl} - \frac{1}{3} \delta_{kl} \bar{\nu}_{qq}) + \delta_{kl}(\bar{\nu}_{ij} - \frac{1}{3} \delta_{ij} \bar{\nu}_{qq})$ , where the first part does not vanish in the incompressible limit. They can be incorporated into the pressure, if the latter is redefined as  $\tilde{p} = p + \bar{\nu}_{kl} A_{kl}$  sacrificing the simple physical meaning of the pressure. According to the symmetries involved there are between zero (in the isotropic and cubic case) and 5 terms (in the triclinic case) of this kind, reducing the number of apparent viscosities further (Table (1)). In (28) the two combinations  $2T_1 + T_4 + T_5$  and  $2T_2 + T_4 + T_6$  give rise to such viscosity contributions, while in (29) there is one additional combination  $T_{10} + T_{11} + T_{12}$  of that kind and 2 more in (30),  $T_{14} + T_{17} + T_{19}$  and  $T_{15} + T_{16} + T_{18}$ .

The director orientational viscosities ( $\gamma$  coefficients) are not affected by the incompressibility assumption. There are 3 of them [13] in orthorhombic biaxial nematics according to the three different rotations involved. For other symmetries their numbers are

listed in Table 1 (in agreement with [14] for the tetragonal and cubic case). The (reactive) flow alignment tensors, on the other hand, are influenced by the incompressibility approximation. Writing the rotations due to elongational flow as [13]

$$\dot{n}_i^{(fa)} = \lambda_{ijk}^{(n)} A_{jk} \quad \dot{m}_i^{(fa)} = \lambda_{ijk}^{(m)} A_{jk} \quad (31)$$

the conditions  $n_i \dot{n}_i = 0 = m_i \dot{m}_i$  and  $n_i m_i = \text{const.}$  require the general form of the  $\lambda$ -tensors to be

$$\begin{aligned} \lambda_{ijk}^{(n)} &= m_i \lambda_{jk}^1 + p_i \lambda_{jk}^2 \\ \lambda_{ijk}^{(m)} &= -n_i \lambda_{jk}^1 + p_i \lambda_{jk}^3 \end{aligned} \quad (32)$$

For orthorhombic symmetry we have 3 coefficients [13] (in Voigt notation)

$$\begin{aligned} \lambda_{ij}^{1,ortho} &= \lambda_{16}(n_i m_j + n_j m_i) \\ \lambda_{ij}^{2,ortho} &= \lambda_{25}(n_i p_j + n_j p_i) \\ \lambda_{ij}^{3,ortho} &= \lambda_{34}(p_i m_j + p_j m_i) \end{aligned} \quad (33)$$

with additional terms in the monoclinic

$$\begin{aligned} \lambda_{ij}^{1,mono} &= \lambda_{ij}^{1,ortho} + \lambda_{11} n_i n_j + \lambda_{12} m_i m_j + \lambda_{13} p_i p_j \\ \lambda_{ij}^{2,mono} &= \lambda_{ij}^{2,ortho} + \lambda_{24}(m_i p_j + m_j p_i) \\ \lambda_{ij}^{3,mono} &= \lambda_{ij}^{3,ortho} + \lambda_{35}(p_i n_j + p_j n_i) \end{aligned} \quad (34)$$

and triclinic case

$$\begin{aligned} \lambda_{ij}^{1,tric} &= \lambda_{ij}^{1,mono} + \lambda_{15}(n_i p_j + n_j p_i) + \lambda_{14}(m_i p_j + m_j p_i) \\ \lambda_{ij}^{2,tric} &= \lambda_{ij}^{2,mono} + \lambda_{21} n_i n_j + \lambda_{22} m_i m_j + \lambda_{23} p_i p_j + \lambda_{26}(n_i m_j + n_j m_i) \\ \lambda_{ij}^{3,tric} &= \lambda_{ij}^{3,mono} + \lambda_{31} n_i n_j + \lambda_{32} m_i m_j + \lambda_{33} p_i p_j + \lambda_{36}(n_i m_j + n_j m_i) \end{aligned} \quad (35)$$

adding up to 3, 8, and 18  $\lambda$  coefficients for the 3 symmetries, respectively. It is easy to see that one term  $\sim \delta_{ij}$  can be constructed each in  $\lambda_{ij}^{1,mono}$ ,  $\lambda_{ij}^{2,tric}$ , and  $\lambda_{ij}^{3,tric}$ , thus reducing the numbers of relevant incompressible  $\lambda$  parameters by 1 and 3 for the monoclinic and triclinic case, respectively (see Table 1) in the incompressible limit.

In the Leslie-Ericksen type description of orthorhombic biaxial nematics 12 (dissipative) transport parameters are found [9] (in the incompressible and isothermal limit). This corresponds to the sum of  $\gamma$  and  $\lambda$  parameters and viscosities  $\nu_p$  and, thus, implies that the pressure in [9] is actually the redefined one,  $\tilde{p}$ . Again the (three) reactive parameters  $\lambda$  are expressed by ratios of dissipative ones. For a Leslie-Ericksen type description of the monoclinic biaxial nematics we can take [22], which was originally intended to describe smectic C liquid crystals with constant layer thickness, i.e. without the compressional mode. However, since 3 different and independent angles are used as dynamic variables, this is applicable to biaxial nematics with monoclinic symmetry, while the smectic C phase has one angle (in-plane rotation of the director structure) and one displacement variable (for layer compression or dilation), from which the two rotation angles of the layer normal are derived (and which are thus not independent) [23]. In [22] 20 transport parameters are found, which again fits nicely with the sum of  $\gamma$  and  $\lambda_{inc}$  parameters and viscosities

$\nu_p$  and, again, implies that the pressure is actually the redefined one,  $\tilde{p}$ . We are not aware of actual Leslie-Ericksen type descriptions of biaxial nematics of triclinic, tetragonal, and cubic symmetry. But we expect the same correspondence to hold between Leslie-Ericksen parameters and hydrodynamic ones as discussed above, and have given the corresponding numbers in Table 1 in parentheses. Obviously, the degree of simplification that is obtained by the incompressibility approximation decreases rapidly with increasing complexity (or decreasing symmetry) of the phase considered.

## 6 Smectic, Columnar and Crystal Phases

We will briefly discuss the notion and consequences of incompressibility in phases with positional order or elasticity. Smectic or layered systems have a one-dimensional, columnar phases a two-dimensional, and crystals a three-dimensional positional order. This constitutes spontaneously broken translational symmetries and the appropriate hydrodynamic symmetry variables are 1-, 2- and 3-dimensional displacement variables  $u_i^{(\alpha)}$  (for complications in the nonlinear theory cf. [23–25]), with  $\alpha = 1, 2, 3$  for smectics, columnar phases and crystals, respectively. They are related to the displacement vector  $u_i$  by  $u_i^{(1)} \equiv k_i k_j u_j$ ,  $u_i^{(2)} \equiv (n_i n_j + m_i m_j) u_j$  and  $u_i^{(3)} \equiv u_i$ , where  $k_i$  is the normal to the smectic layers, and  $n_i$ ,  $m_i$  are the preferred directions of the 2D lattice of the columns. Only where necessary we will discriminate between smectic A ( $D_{\infty h}$  symmetry) and smectic C ( $C_{2h}$ ), and between orthorhombic ( $D_{2h}$ ), tetragonal ( $D_{4h}$ ) and hexagonal ( $D_{6h}$ ) columnar phases.

The linearized dynamic equation for the elastic degree of freedom can be written [11, 13, 17] (neglecting a dissipative crosscoupling to temperature gradients)

$$\dot{u}_i^{(\alpha)} - v_i^{(\alpha)} = \xi_{ij}^{(\alpha)} \nabla_k \phi_{jk}^{(\alpha)} \quad (36)$$

where  $v_i^{(\alpha)}$  is related to the velocity  $v_i$  in the same way as  $u_i^{(\alpha)}$  to  $u_i$ . It should be noted that in the Eulerian description  $u_i$  is not the position vector of a particle and therefore its time derivative is not identical to the velocity (of a particle). The difference between the time derivative of the displacement field and the velocity field is due to a dissipative process known as permeation in smectics and columnar phases and called vacancy diffusion in solids [11]. The permeation tensor  $\xi_{ij} = \xi k_i k_j$  has one coefficient in smectic systems, generally two  $\xi_{ij} = \xi_1 n_i n_j + \xi_2 m_i m_j$  in columnar systems (with  $\xi_1 = \xi_2$  for tetragonal and hexagonal symmetry) and 1 to 6 coefficients (like the dielectric tensor) in crystals depending on their symmetry. The elastic stress  $\phi_{ij}^{(\alpha)}$  follows from the free energy  $F$  by differentiation

$$\phi_{ij}^{(\alpha)} \equiv \frac{\delta F}{\delta \nabla_j u_i^{(\alpha)}} = c_{ijkl}^{(\alpha)} \nabla_k u_l^{(\alpha)} - K_{ijklmn}^{(\alpha)} \nabla_k \nabla_l \nabla_m u_n^{(\alpha)} \quad (37)$$

containing Hooke's law as well as curvature effects. In smectics there is only a 1-dimensional compression or dilation  $c_{ijkl}^{(1)} = B_0 k_i k_j k_k k_l$ , while in columnar phases also in-plane shear stresses are possible [13]

$$\begin{aligned} c_{ijkl}^{(2)} = & c_1 n_i n_j n_k n_l + c_2 m_i m_j m_k m_l + c_4 (n_i n_j m_k m_l + n_k n_l m_i m_j) \\ & + c_3 (n_i n_k m_j m_l + n_i n_l m_j m_k + n_j n_k m_i m_l + n_j n_l m_i m_k) \end{aligned} \quad (38)$$

with  $c_1 = c_2$  for the tetragonal, and, additionally,  $c_3 = c_1 - c_4$  for the hexagonal, case. For crystals  $c_{ijkl}^{(3)} = c_{ijkl}$  is the usual elastic tensor. For the latter case curvature effects are almost always neglected, while for smectics

$$K_{ijklmn}^{(1)} = k_i k_n (\delta_{jk} - k_j k_k) (K_1 (\delta_{lm} - k_l k_m) + K_3 k_l k_m) \quad (39)$$

there is layer bend (= director splay) and layer splay (= director bend) expressed by  $K_1$  and  $K_3$ , respectively. For the columnar case we refer to [26].

Incompressibility again means constant density in time and space resulting in  $div \mathbf{v} = 0$  and is obtained for vanishing compressibility and thermal expansion. The compatibility condition for the pressure, which ensures  $div \mathbf{v} = 0$  for all times, now involves the elastic stresses

$$\Delta p = \nabla_i \nabla_j \phi_{ij}^{(\alpha)} + \nu_{ijkl} \nabla_i \nabla_j A_{kl} \quad (40)$$

The consequences of incompressibility for the viscosity tensor depend on the symmetry of the phases under consideration and has been discussed in the previous sections.

In the smectic and columnar case there are no effects due to incompressibility for the displacement field  $u_i^{(1,2)}$  nor for its time derivative  $\dot{u}_i^{(1,2)}$ . Here  $div \mathbf{v} = 0$  does neither imply  $div \mathbf{v}^{(1,2)} = 0$  (nor  $div \dot{\mathbf{u}}^{(1,2)} = 0$ ), but rather that these (1D or 2D compressional) flows are compensated by transverse (dilational) flows, since  $\nabla_i v_i^{(1,2)} = -\delta_{ij}^{tr1,2} \nabla_i v_j \neq 0$  with  $\delta_{ij}^{tr1} = \delta_{ij} - k_i k_j$  and  $\delta_{ij}^{tr2} = \delta_{ij} - n_i n_j - m_i m_j$ . In smectics sometimes the assumption of constant layer spacing ("layer incompressibility") is made, which then allows only curvature of the layers. This has nothing to do with the incompressibility condition  $div \mathbf{v} = 0$ , but is obtained by the *additional* assumption of an infinite layer-compression modulus,  $B_0 \rightarrow \infty$ , which implies  $(\mathbf{k} \cdot \nabla)^n \mathbf{u}^{(1)} \equiv 0$  for  $n \geq 1$ . This in turn restricts the velocity field in (36) to obey  $\nabla_i v_i^{(1)} = k_i k_j \nabla_j v_i = 0$ . This condition is difficult to implement in actual problems and makes treatments with  $B_0 \rightarrow \infty$  rather dubious. Similar considerations apply to columnar phases.

Somewhat different is the case of crystals. Here  $div \mathbf{v} = 0$  requires the compatibility condition via (36)

$$\nabla_i \dot{u}_i = \xi_{ij} c_{jklm} \nabla_i \nabla_k \nabla_l u_m \quad (41)$$

showing that  $div \mathbf{u} \neq 0$ , generally. Only if vacancy diffusion is neglected additionally,  $\xi_{ij} = 0$ ,  $div \mathbf{u} = 0$  is obtained. That additional assumption is inherent to all continuum theoretical treatments based on the Lagrangian approach, where  $div \mathbf{u} = -\delta\rho/\rho$  [18], which gives  $div \mathbf{u} = 0$  in the incompressible limit. If vacancy diffusion is not neglected,  $div \mathbf{u} = 0$  is a solution of (41) in the isotropic case (disordered solids), only. In that case the bulk elastic modulus drops out automatically from the elastic stress  $\phi_{ij}$  and thus also from the dynamics. However, even for the simplest crystal symmetry, the cubic one (and of course for all more complicated ones),  $div \mathbf{u} = 0$  is *not* a solution of (41) and all three (or more) elastic moduli remain relevant despite the incompressibility assumption.

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