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Poisson-bracket approach to the dynamics of nematic liquid crystals

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We use the general Poisson-bracket formalism for obtaining stochastic dynamical equations for slow macroscopic fields to derive the equations that govern the dynamics of nematic liquid crystals in both their nematic and isotropic phases. For uniaxial molecules, we calculate the Poisson bracket between the tensorial nematic order parameter $\boldsymbol{Q}$ and the momentum density $\boldsymbol{g}$, as well as those between all pairs of conserved quantities. We show that the full nonlinear hydrodynamical equations for the nematic phase derived in this formalism are identical to the nonlinear Ericksen-Leslie equations. We also obtain the complete dynamical equations for the slow dynamics of the tensorial nematic order parameter $\boldsymbol{Q}$ valid both in the isotropic and the nematic phase. They differ from those obtained by other techniques only in the values of kinetic coefficients and in the number of nonlinear terms in $\boldsymbol{Q}$, which are present.

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I. INTRODUCTION

Nematic liquid crystals are unique materials, since they flow in all directions such as a homogeneous fluid and yet they are optically anisotropic [1,2]. Their low-frequency dynamical properties, which are characterized by orientational relaxation as well as by shear and compressional flow [3–5], are central to the switching behavior of liquid crystal displays [6]. They give rise to interesting fundamental phenomena including electrohydrodynamical pattern formation [7], instabilities under shear flow [1,2], orientational fluctuations observable in light scattering experiments [8], and the anisotropic and nonlinear Stokes drag on a particle embedded in a nematic solvent [9]. Nematic liquid crystals raise fundamental questions about how broken symmetries affect low-frequency hydrodynamics, and it is not surprising that over the years there have been a number of derivations [3–5,1] of the equations governing nematohydrodynamics. In this paper, we present a derivation of these equations, and of the equations governing the relaxation of the symmetric-traceless-tensor nematic order parameter $\boldsymbol{Q}$ [10–12,1] in both the nematic and the isotropic phase. We use the Poisson-bracket formalism of classical mechanics [13] developed in the framework of stochastic equations for fluctuating macroscopic field variables [14–18] and applied to dynamical critical phenomena [19].

Using the formalism of rational mechanics, Ericksen and Leslie were the first to derive a full set of dynamic equations, commonly referred to as Ericksen-Leslie equations [3,4], for the velocity and director field $\boldsymbol{n}$ specifying the direction of nematic anisotropy. Later, the Harvard group argued that the interpretation of the dynamic equation for the director (the so-called Oseen equation) as the balance law for the angular momentum is not well justified [20], and they presented a rigorous derivation of the linearized hydrodynamic equations starting from conserved and hydrodynamic Goldstone variables [5]. The full nonlinear theory based on this apprach was developed by Pleiner and Brand [21]. De Gennes pointed out the common features of the two approaches [1]. Recently, Sonnet and Virga rederived the Ericksen-Leslie equations in the framework of a variational principle of Rayleigh starting from complex fluids with a general tensorial order parameter [22].

The low-frequency hydrodynamics of the nematic phase is determined entirely by the conserved densities, characterizing both the isotropic and nematic phases, and the director $\boldsymbol{n}$. There are, however, physical situations in which the director alone does not provide a complete description of the nematic orientational order, and a description in terms of the full nematic order parameter $\boldsymbol{Q}$ (also called the alignment tensor [23]) is required. As a result, there has been an increasing interest in dynamical equations both in the nematic and the isotropic phases in which the nematic order is described by $\boldsymbol{Q}$ rather than by $\boldsymbol{n}$ alone. These equations necessarily include nonhydrodynamic modes, which nonetheless have characteristic relaxation times that are slow compared to microscopic times. In conjunction with the Landau-Ginzburg–de Gennes free energy, they provide a description of dynamical processes close to the nematic-isotropic phase transition [23–26], of processes in which the degree of ordering can vary, e.g., by applying a shear deformation, or of processes in thin liquid crystal cells subject to large external fields [27]. They also provide a detailed description of the dynamics of line and point defects [28,29] whose cores exhibit a complex biaxial ordering which is beyond the simple director picture [30].

The first complete formulation of the dynamic equations involving the $\boldsymbol{Q}$ tensor was presented by Hess [23]. Subsequent refinements were carried out by Kuzuu and Doi, who started from a molecular kinetic equation [31], and by Olmsted and Goldbart [25], who set up the dynamic equations in full analogy to de Gennes's derivation of the Ericksen-Leslie theory in Ref. [1]. In parallel, Edwards, Beris, and Grmela pioneered a derivation based on a Hamiltonian formulation of continuum mechanics [32]. Further approaches to the $\boldsymbol{Q}$ tensor dynamics are introduced in Ref. [27] by Qian and Sheng, in Ref. [22] by Sonnet and Virga, and in Ref. [33] by Pleiner, Liu, and Brand. The latter though purely phenomenological is very close in spirit to the approach we present here.

The Poisson-bracket approach we adopt in this paper has several advantages. First, it automates the derivation of

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coarse-grained dynamical equations once the dynamic field variables are defined. As we shall see in the following, this approach, however, requires more carefulness in nematic liquid crystals than it does in other systems such as magnets and superfluids. Second, the formalism applies to nonhydrodynamic slow variables as well as to true hydrodynamic variables. Third, it gives easy access to nonlinear terms, as they appear, e.g., in the convective derivative of the Navier-Stokes equations. The formalism has been applied to diverse systems such as (anti)ferromagnets [19], quasicrystals [34], or to nematic polymers [35] which demonstrate its universality.

In the literature, different methods are used to calculate the Poisson brackets. Volovik employs pure symmetry arguments [36,37] that are not sufficient to provide a full description of nematic liquid crystals because it fails to properly treat the degree of nematic ordering. Edwards, Beris, and Grmela on the other hand define their Poisson brackets on a continuum level [38].

Here, in contrast, we start from a microscopic definition of the field variables. Following the work of Forster [39], we introduce such variables for model-liquid-crystal molecules made from point particles and employ the conventional definition from classical mechanics to arrive at coarse-grained Poisson brackets for the macroscopic field variables. A careful treatment is needed to determine the central Poisson bracket between the alignment tensor $\boldsymbol{Q}$ and the momentum density which extends the work of Forster [39]. We then rederive the Ericksen-Leslie theory and rigorously justify the Oseen equation. The Onsager and Parodi relations for the Leslie viscosities are automatically fulfilled [40]. We derive generalized dynamic equations for the alignment tensor. Our equations have the same form as those derived by Olmsted and Goldbart [25] and those obtained by Pleiner *et al.* [33]. We obtain explicit forms for reactive coefficients that are merely unspecified phenomenological coefficients in these approaches. Our equations have terms not present in those of Olmsted and Goldbart, and those of Pleiner *et al.* contain nonlinear terms that our equations do not.

The paper is organized as follows. In Sec. II, we introduce the general formalism. In Sec. III, we define the molecular model and calculate all relevant Poisson brackets. The full sets of dynamic equations for the director or the $\boldsymbol{Q}$-tensor dynamics are derived and discussed in Secs. IV and V, respectively.

II. GENERAL FORMALISM

In this section, we summarize the general formalism on which our derivation of the dynamic equations in nematic liquid crystals is based. Let us consider systems whose microscopic dynamics is determined by canonically conjugate variables $\boldsymbol{x}^\alpha$ and $\boldsymbol{p}^\alpha$ for each particle α and a microscopic Hamiltonian $\hat{\mathcal{H}}(\{\boldsymbol{x}^\alpha\},\{\boldsymbol{p}^\alpha\})$, where $\{\boldsymbol{x}^\alpha\}=\boldsymbol{x}^1,\boldsymbol{x}^2,\ldots$ etc. Here, we focus on a set of macroscopic field variables $\Phi_\mu(\boldsymbol{x},t)$ for $\mu=1,2,\ldots$ obtained from microscopic fields $\hat{\Phi}_\mu(\boldsymbol{x},\{\boldsymbol{x}^\alpha\},\{\boldsymbol{p}^\alpha\})$ by coarse graining over spatial fluctuations on the microscopic level; $\Phi_\mu(\boldsymbol{x},t)=[\hat{\Phi}_\mu(\boldsymbol{x},\{\boldsymbol{x}^\alpha\},\{\boldsymbol{p}^\alpha\})]_c$, where the symbol $[\cdots]_c$ specifies the coarse-grained averages. The statistical mechanics of the fields $\Phi_\mu(\boldsymbol{x},t)$ is determined by the coarse-grained Hamiltonian $\mathcal{H}[\{\Phi_\mu\}]$, which is a functional of the macroscopic variables. It is constructed in such a way that the statistical averages of observables in the microscopic and the macroscopic representation are identical. In formulas, this means

$$\begin{aligned}\langle f(\{\hat{\Phi}_\mu\})\rangle &= \int \mathcal{D}(\boldsymbol{x}^\alpha,\boldsymbol{p}^\alpha) f(\{\hat{\Phi}_\mu\}) e^{-\hat{\mathcal{H}}/k_{\mathrm{B}}T}\\ &\equiv \langle f(\{\Phi_\mu(\boldsymbol{x},t)\})\rangle\\ &= \int \mathcal{D}\Phi_\mu(\boldsymbol{x},t) f(\{\Phi_\mu(\boldsymbol{x},t)\}) e^{-\mathcal{H}/k_B T},\end{aligned}$$

where k_B is the Boltzmann constant, T is the temperature, and $\mathcal{D}(\boldsymbol{x}^\alpha,\boldsymbol{p}^\alpha)$ and $\mathcal{D}\Phi_\mu(\boldsymbol{x},t)$ are integration measures. The observable f is a function of the microscopic ($\hat{\Phi}_\mu$) or macroscopic (Φ_μ) fields. In practice, phenomenological forms for $\mathcal{H}[\{\Phi_\mu\}]$ are used.

The macroscopic fields $\Phi_\mu(\boldsymbol{x},t)$ describe the slow dynamic response of the system, i.e., they are either hydrodynamic or quasihydrodynamic variables whose characteristic decay times τ in the long-wavelength limit are much larger than microscopic decay times. Then, following the theory of kinetic or stochastic equations, the variables evolve according to [17–19]

$$\frac{\partial \Phi_\mu(\boldsymbol{x},t)}{\partial t} = V_\mu(\boldsymbol{x}) - \Gamma_{\mu\nu}\frac{\delta \mathcal{H}}{\delta \Phi_\nu(\boldsymbol{x})}, \tag{1}$$

where the reactive term $V_\mu(\boldsymbol{x})$ is also called nondissipative or streaming velocity and the second term introduces dissipative effects. These equations, which can be rigorously derived from microscopic principles following the works by Zwanzig [14], Kawasaki [15], and Mori, Fujisaka, and Shigematsu [16], describe the low-frequency and the long-wavelength dynamics of the system. When applied to an isotropic fluid, for example, they correctly reproduce the fully nonlinear Navier-Stokes equations. Supplemented with a noise term $\zeta_\mu(\boldsymbol{x},t)$, they provide a powerful formalism for calculating dynamical correlation functions in equilibrium and, especially, for treating effects due to the coupling between modes. As such, the stochastic equations are used extensively in the study of dynamical critical phenomena, where nonlinearities are important [19]. In this paper, we are mainly interested in deriving the equations for the low-frequency dynamics of the isotropic and nematic phases of liquid crystals, and we will not give any further consideration to the noise. Disregarding noise in Eq. (1) means that nonequilibrium averages of the macroscopic field variables are used [41].

The concrete form of the reactive term involves Poisson brackets which are the central quantity of this formalism; it can be expressed as

$$V_\mu(\boldsymbol{x}) = -\int d^3x' \mathcal{P}_{\mu\nu}(\boldsymbol{x},\boldsymbol{x}')\frac{\delta \mathcal{H}}{\delta \Phi_\nu(\boldsymbol{x}')}, \tag{2}$$

where Einstein's convention on repeated indices is understood and

$$\mathcal{P}_{\mu\nu}(\boldsymbol{x},\boldsymbol{x}')=\{\Phi_\mu(\boldsymbol{x}),\Phi_\nu(\boldsymbol{x}')\}=-\mathcal{P}_{\nu\mu}(\boldsymbol{x}',\boldsymbol{x}) \tag{3}$$

denotes the Poisson bracket of the coarse-grained variables. It is defined as the coarse-grained average of the microscopic Poisson bracket:

$$\{\Phi_\mu(\boldsymbol{x}),\Phi_\nu(\boldsymbol{x}')\}=[\{\hat{\Phi}_\mu(\boldsymbol{x}),\hat{\Phi}_\nu(\boldsymbol{x}')\}]_c, \tag{4}$$

where [13]

$$\{\hat{\Phi}_\mu(\boldsymbol{x}),\hat{\Phi}_\nu(\boldsymbol{x}')\}=\sum_{\alpha i}\frac{\partial\hat{\Phi}_\mu(\boldsymbol{x})}{\partial p_i^\alpha}\frac{\partial\hat{\Phi}_\nu(\boldsymbol{x}')}{\partial x_i^\alpha}-\frac{\partial\hat{\Phi}_\mu(\boldsymbol{x})}{\partial x_i^\alpha}\frac{\partial\hat{\Phi}_\nu(\boldsymbol{x}')}{\partial p_i^\alpha}. \tag{5}$$

Equation (2) can be rigorously derived from microscopic principles [14–16]. Roughly speaking, it can be viewed as the Poisson bracket $\{\mathcal{H},\Phi_\mu\}$ which in classical mechanics describes the time evolution of an observable [13]. Applying the chain rule to the derivatives of the Hamiltonian and noting that Φ_ν is a field variable, the formal structure of Eq. (2) results. However, since we only employ a restricted number of coarse-grained macroscopic variables, all the "neglected" microscopic degrees of freedom give rise to the dissipative term in the kinetic equation (1). It is proportional to the generalized force $\delta\mathcal{H}/\delta\Phi_\nu(\boldsymbol{x})$ which together with $\Phi_\nu(\boldsymbol{x})$ forms a pair of conjugate variables. The quantity $\Gamma_{\mu\nu}$ is called the dissipative tensor that, in general, may depend on the fields Φ_μ and that may also contain terms proportional to $-\boldsymbol{\nabla}^2$. It is determined by three principles. First, $\partial\Phi_\mu/\partial t$ can only couple to $\delta\mathcal{H}/\delta\Phi_\nu$ if it possesses a different sign under time reversal, the signature of dissipation. Second, $\Gamma_{\mu\nu}$ has to reflect the local point group symmetry of the dynamic system, and third, it has to be a symmetric tensor at zero magnetic field to obey the Onsager principle [42].

III. POISSON BRACKETS FOR NEMATIC LIQUID CRYSTALS

Our goal is to use the formalism outlined above to derive the dynamical equations for the long-lived fields in a nematic liquid crystal and the isotropic phase from which the nematic phase develops. Our most important results are the Poisson brackets of Eqs. (4) and (5), which we will derive in this section starting from an explicit microscopic model for the constituent molecules.

Conserved fields are always hydrodynamical variables because their frequencies necessarily tend to zero with wave number. In systems with a continuous broken symmetry, there are additional broken-symmetry hydrodynamical variables. In addition, there can be modes that have characteristic decay times that are much longer than any microscopic times even though they do not tend to infinity with wave number. The conserved variables of both the isotropic and nematic phases are the mass density $\rho(\boldsymbol{x},t)$, the momentum density $\boldsymbol{g}(\boldsymbol{x},t)$, and the energy density $\epsilon(\boldsymbol{x},t)$, where the latter quantity will not be considered further in this paper. In the nematic phase, the Frank director $\boldsymbol{n}(\boldsymbol{x},t)$ is the broken-symmetry hydrodynamical variable with two independent degrees of freedom. As long as there are no topological defects present, it is sufficient to describe the dynamics of the orientational order by $\boldsymbol{n}(\boldsymbol{x},t)$. Otherwise, one has to resort to a more general order parameter that is able to quantify, e.g., the biaxial ordering in the core of a topological defect. We will describe nematic order with the conventional Saupe–de Gennes second-rank symmetric-traceless tensor parameter $\boldsymbol{Q}(\boldsymbol{x},t)$ [10–12,1], also called alignment tensor [23]. In the isotropic phase, especially near the isotropic-to-nematic transition, $\boldsymbol{Q}(\boldsymbol{x},t)$ can be a slow variable whose relaxation to equilibrium is much slower than any microscopic collision time. In the nematic phase, it also contains slow, nonhydrodynamic components in addition to the hydrodynamic director variable.

The complexity of nematic order presents problems not encountered in many other broken-symmetry systems such as magnets and superfluids. Nematic order is associated with local molecular rigidity, and it only arises if constituent molecules are anisotropic. A central quantity in our formalism are the Poisson brackets between the alignment tensor $\boldsymbol{Q}(\boldsymbol{x},t)$ or the director $\boldsymbol{n}(\boldsymbol{x},t)$ and the momentum density $\boldsymbol{g}(\boldsymbol{x},t)$. However, in the following it will become obvious that the calculation of these Poisson brackets is not straightforward since neither the nematic order parameter $\boldsymbol{Q}$ nor the director $\boldsymbol{n}$ can be defined as simple coarse-grained averages of microscopic quantities.

A. Model molecule and dynamic variables

Our system contains a number of identical model-liquid-crystal molecules indexed by α, which consist of a set of mass points with masses m^μ and position vectors $\boldsymbol{x}^{\alpha\mu}$. We also introduce position vectors $\Delta\boldsymbol{x}^{\alpha\mu}=\boldsymbol{x}^{\alpha\mu}-\boldsymbol{x}^\alpha$ relative to the location of the center of mass of each molecule at $\boldsymbol{x}^\alpha=\Sigma_\mu(m^\mu\boldsymbol{x}^{\alpha\mu})/m_0$, where $m_0=\Sigma_\mu m^\mu$ is the total mass of a molecule. In our derivation of the Poisson brackets, it is important that the molecules are not rigid, but that their constituent atoms be allowed to fluctuate around their average positions. For simplicity, we will assume that the molecules have a uniaxial shape in the sense that their moment of inertia tensor, to be defined below, is also uniaxial. Considering the fact that molecules perform fast rotations about their long axis on a time scale of 10^{-10} s [43], this is not a very severe restriction. With our model we can describe a huge range of possible molecules ranging from needlelike objects to molecules with prolate and oblate (disklike) shape. Even globular polymers with anisotropic shape are included.

We employ the conventional microscopic definition of the density of mass and momentum:

$$\hat{\Phi}_1=\hat{\rho}(\boldsymbol{x})=\sum_{\alpha\mu}m^\mu\delta(\boldsymbol{x}-\boldsymbol{x}^{\alpha\mu}), \tag{6}$$

$$\hat{\Phi}_{2-4}=\hat{\boldsymbol{g}}(\boldsymbol{x})=\sum_{\alpha\mu}\boldsymbol{p}^{\alpha\mu}\delta(\boldsymbol{x}-\boldsymbol{x}^{\alpha\mu}), \tag{7}$$

which, after coarse graining, result in the macroscopic variables $\rho(\boldsymbol{x})=[\hat{\rho}(\boldsymbol{x})]_c$ and $\boldsymbol{g}(\boldsymbol{x})=[\hat{\boldsymbol{g}}(\boldsymbol{x})]_c$. Note that the δ function has the dimension of an inverse volume. We stress that the definition of the momentum density in Eq. (7) includes the motion of all mass points, including, in particular, rotational motion about the centers of mass of anisotropic particles.

To describe the orientational order of the molecules, we follow the approach of Forster [39] who extracted the anisotropic part from the density of the moment-of-inertia tensor and used its negative part as an additional microscopic field variable:

$$\hat{R}_{ij}(\boldsymbol{x})=\sum_\alpha \hat{R}^\alpha_{ij}\,\delta(\boldsymbol{x}-\boldsymbol{x}^\alpha), \tag{8}$$

where for each molecule α we have

$$\hat{R}^\alpha_{ij}=\sum_\mu m^\mu\left[\Delta x_i^{\alpha\mu}\Delta x_j^{\alpha\mu}-\tfrac{1}{3}(\Delta x_k^{\alpha\mu})^2\delta_{ij}\right]. \tag{9}$$

The coarse-grained variable $\boldsymbol{R}(\boldsymbol{x})=[\hat{\boldsymbol{R}}(\boldsymbol{x})]_c$ is a symmetric and traceless tensor of second rank, as demanded for the nematic order parameter $\boldsymbol{Q}(\boldsymbol{x})$, but it also depends on the density of the molecules and, more important, it includes the fast fluctuations of the molecules around their average configuration, which we are not interested in. To arrive at an expression for $\boldsymbol{Q}(\boldsymbol{x})$, we note that $\hat{R}^\alpha_{ij}$ is a tensor that for any particular atomic configuration can be represented in a basis in which it is diagonal. Since this tensor is traceless, it has only two independent eigenvalues, one of which describes molecular biaxiality. Here, we will consider only molecules that are, on an average, uniaxial. In any real molecule, there will be fluctuations in which it becomes momentarily biaxial. We assume, however, that these fluctuations relax rapidly in nonhydrodynamic times. In this case, $\hat{R}^\alpha_{ij}$ is characterized by a single parameter in addition to the unit vector $\hat{\boldsymbol{\nu}}^\alpha$ its largest-eigenvalue principal axis. Then

$$\hat{R}^\alpha_{ij}=R^\alpha Q^\alpha_{ij}, \tag{10}$$

where

$$Q^\alpha_{ij}=\hat{\nu}^\alpha_i\hat{\nu}^\alpha_j-\frac{1}{3}\delta_{ij} \tag{11}$$

is the local molecular alignment tensor and R^α will be given below. When this form of $\hat{R}^\alpha_{ij}$ is valid, we can define the coarse-grained position dependent Saupe–de Gennes order parameter via

$$R_{ij}(\boldsymbol{x})=\left[\sum_\alpha \hat{R}^\alpha_{ij}\,\delta(\boldsymbol{x}-\boldsymbol{x}^\alpha)\right]_c=R(\boldsymbol{x})Q_{ij}(\boldsymbol{x}), \tag{12}$$

where

$$R(\boldsymbol{x})\equiv[\hat{R}(\boldsymbol{x})]_c=\left[\sum_\alpha R^\alpha\,\delta(\boldsymbol{x}-\boldsymbol{x}^\alpha)\right]_c. \tag{13}$$

The nematic order parameter $Q_{ij}(\boldsymbol{x})$ must reduce to $n_in_j-\frac{1}{3}\delta_{ij}$ when all local axes $\hat{\boldsymbol{\nu}}^\alpha$ are aligned along the spatially uniform director $\boldsymbol{n}$, and all molecules have the same value of R^α. It is straightforward to verify that the tensor $Q_{ij}(\boldsymbol{x})$ defined in Eq. (12) satisfies this constraint. Note that the fields $Q_{ij}(\boldsymbol{x})$ constitute the fields $\Phi_{5-9}(\boldsymbol{x})$ in our formalism.

The parameter R^α can easily and usefully be related to the anisotropy in the molecular moment-of-inertia tensor

$$I^\alpha_{ij}=\sum_\mu m^\mu\left[(\Delta x^{\alpha\mu})^2\delta_{ij}-\Delta x_i^{\alpha\mu}\Delta x_j^{\alpha\mu}\right], \tag{14}$$

whose components parallel and perpendicular to the local anisotropy axis $\hat{\boldsymbol{\nu}}^\alpha$ in a *uniaxial* system are, respectively,

$$I^\alpha_\parallel=\sum_\mu m^\mu(\Delta\boldsymbol{x}_\perp^{\alpha\mu})^2, \tag{15}$$

$$I^\alpha_\perp=\sum_\mu m^\mu\left[(\Delta\boldsymbol{x}_\perp^{\alpha\mu})^2/2+(\Delta x_\parallel^{\alpha\mu})^2\right], \tag{16}$$

where $\Delta\boldsymbol{x}_\perp^{\alpha\mu}$ and $\Delta x_\parallel^{\alpha\mu}$ are, respectively, the component of $\Delta\boldsymbol{x}^{\alpha\mu}$ parallel and perpendicular to $\hat{\boldsymbol{\nu}}^\alpha$. The anisotropy ΔI^α distinguishes between prolate ($\Delta I^\alpha>0$) and oblate ($\Delta I^\alpha<0$) molecules. For uniaxial systems, we find

$$R^\alpha=\Delta I^\alpha\equiv I^\alpha_\perp-I^\alpha_{||}. \tag{17}$$

Only after calculating the Poisson brackets (see Sec. III C), can we safely replace R^α by its averaged value ΔI, since, in microscopic times, R^α of different molecules relax to the same value ΔI. In this case, we can replace $R(\boldsymbol{x})$ with

$$R(\boldsymbol{x})=\frac{\Delta I}{m_0}\rho(\boldsymbol{x}). \tag{18}$$

Then, Eq. (12) results in the conventional definition of $Q_{ij}(\boldsymbol{x})$, where Q^α_{ij} [see Eq. (11)] is averaged over many molecules. In what follows, we will also use

$$\mathrm{Tr}\,\boldsymbol{I}^\alpha=I=I_{||}+2I_\perp, \tag{19}$$

where the final form is in the uniaxial case we consider when all fast modes have relaxed.

We stress that our approach is a generalization of the one describing a simple flexible diatomic molecule in which the principal moments of inertia fluctuate and therefore have a nonvanishing Poisson bracket with the momentum density. Our quantity $\hat{R}(\boldsymbol{x})$ incorporates these fluctuations for a more complex molecule. As we will see below, the Poisson brackets of $\hat{R}(\boldsymbol{x})$ with the momentum density will give rise to one additional term in the analogous Poisson brackets of $\boldsymbol{Q}(\boldsymbol{x})$. This essential contribution was not taken into account by Forster [39] who considered $R(\boldsymbol{x})$ as a constant. Instead, $\hat{R}(\boldsymbol{x})$ is a dynamic quantity since it depends on the mass density of the molecules through the δ functions in Eq. (13) and, more importantly, also reflects the fluctuations in the anisotropy R^α of the molecular moment of inertia tensor. Whereas the dependence on the mass density only produces a term in the Poisson brackets of $\boldsymbol{Q}(\boldsymbol{x})$, which is irrelevant for incompressible fluids, the fluctuations in R^{α} give rise to the essential contribution just mentioned.

B. Poisson brackets

In calculating the Poisson brackets according to Eq. (5), we use the following properties of the δ function:

$$\delta(\boldsymbol{x}-\boldsymbol{x}')=\delta(\boldsymbol{x}'-\boldsymbol{x}), \tag{20a}$$

$$f(\boldsymbol{x})\,\delta(\boldsymbol{x}-\boldsymbol{x}')=f(\boldsymbol{x}')\,\delta(\boldsymbol{x}-\boldsymbol{x}'), \tag{20b}$$

$$\nabla_i\,\delta(\boldsymbol{x}-\boldsymbol{x}')=-\nabla_i'\,\delta(\boldsymbol{x}-\boldsymbol{x}'), \tag{20c}$$

where $\nabla_i=\partial/\partial x_i$, $\nabla_i{}'=\partial/\partial x_i'$ and $f(\boldsymbol{x})$ is an arbitrary function including the δ function itself. Furthermore, we employ the antisymmetry relation of Eq. (3).

In the following, we list all the Poisson brackets with a nonzero value, briefly explain their meaning, and comment on their consequences. The evaluation of the Poisson brackets is straightforward, except for $\{Q_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\}$ which we illustrate in the following subsection.

We start with the dynamics of the mass density $\rho(\boldsymbol{x})$ for which we need

$$\{\rho(\boldsymbol{x}),g_i(\boldsymbol{x}')\}=\nabla_i\delta(\boldsymbol{x}-\boldsymbol{x}')\rho(\boldsymbol{x}'). \tag{21}$$

Using the kinetic part of the Hamiltonian, $\int d^3x\, g^2/(2\rho)$, and the definition of velocity, $v_i=\delta\mathcal{H}/\delta g_i=g_i/\rho$, the dissipative velocity from Eq. (2) results in $V_1(\boldsymbol{x})=V^{\rho}(\boldsymbol{x})=-\nabla_i g_i(\boldsymbol{x})$. Since the the mass-conservation law does not allow for a dissipative contribution ($\Gamma_{1\nu}=0$), we arrive at $\partial\rho/\partial t=-\mathrm{div}\boldsymbol{g}(\boldsymbol{x})$.

For the dynamics of the alignment tensor, we need the Poisson bracket of $Q_{ij}(\boldsymbol{x})$ with $g_k(\boldsymbol{x})$. In agreement with general phenomological arguments [33], we find that this Poisson bracket can be expressed as

$$\{Q_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\}=[\nabla_k Q_{ij}(\boldsymbol{x})]\,\delta(\boldsymbol{x}-\boldsymbol{x}')-\lambda_{ijkl}(\boldsymbol{x})\nabla_l\delta(\boldsymbol{x}-\boldsymbol{x}'). \tag{22}$$

Its derivation is illustrated in Sec. III C. λ_{ijkl} depends on the order parameter Q_{ij}, and in our calculation it is given by

$$\begin{aligned}\lambda_{ijkl}={}&\frac{1}{2}(\delta_{ik}Q_{jl}-\delta_{il}Q_{jk}+\delta_{jk}Q_{il}-\delta_{jl}Q_{ik})\\&+\frac{I}{6\Delta I}\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\tfrac{2}{3}\,\delta_{ij}\delta_{kl}\right)\\&+\frac{1}{2}(\delta_{ik}Q_{jl}+\delta_{il}Q_{jk}+\delta_{jk}Q_{il}+\delta_{jl}Q_{ik}-\tfrac{4}{3}\delta_{ij}Q_{kl})\\&-\frac{2}{3}\delta_{kl}Q_{ij}-\left(1+\frac{I}{2\Delta I}\right)Q_{ij}Q_{kl}.\end{aligned} \tag{23}$$

Note that $\lambda_{iikl}=0$ since $Q_{ii}=0$. In deriving Eqs. (22) and (23), we have omitted derivative terms of order $\boldsymbol{\nabla\nabla}$ and higher. In the nondissipative velocity for $\boldsymbol{Q}$, the first term on the right-hand side of Eq. (22) produces the convective derivative $v_k\nabla_k Q_{ij}$, and the second term gives rise to a reactive coupling to $\nabla_l v_k$. All but the last term of λ_{ijkl} in Eq. (23) were basically derived by Forster in Ref. [39]. Since he did not take into account the dynamics of the scalar variable $R(\boldsymbol{x})$, he missed the second-order term in $\boldsymbol{Q}$ that results from the dynamics of the anisotropy R^{α}. Furthermore, the prefactor of the term $Q_{ij}\delta_{kl}$ was -1. Note that this expression $Q_{ij}\delta_{kl}$ is irrelevant for incompressible fluids. The term in the first line of Eq. (23) is the only one that is antisymmetric under interchange of *k* and *l*. Its form is entirely dictated by rotational symmetry, and there can be no other terms antisymmetric in *k* and *l*. The prefactors depending on $I/\Delta I$ in the second and fourth lines reduce, respectively, to 1/3 and 2 in the case of an infinitely thin needle. Our form of λ_{ijkl} agrees with that determined by Pleiner, Liu, and Brand [33] using phenomenological symmetry arguments. Their expression, however, contains five additional terms of second order in $\boldsymbol{Q}$, which our calculations do not produce. In addition, we find specific values for the coefficients of the second through the fourth lines of Eq. (23), which they view as phenomenological parameters. The more general form considered by Pleiner *et al.* is clearly permitted by symmetry, and one can ask how it can arise from a microscopic model. It is almost certain that mode coupling will renormalize our coefficients and produce the additional terms of second order in $\boldsymbol{Q}$, but it is difficult at this point to estimate how large these mode-coupling corrections would be. It is also possible that molecular biaxiality will lead to additional second-order terms; we have not investigated this question in detail. In what follows, we will continue to use the specific form produced by our Poisson-bracket calculation.

Finally, several nondissipative terms for the momentum balance equation follow from

$$\{g_i(\boldsymbol{x}),\rho(\boldsymbol{x}')\}=\rho(\boldsymbol{x})\nabla_i\delta(\boldsymbol{x}-\boldsymbol{x}'), \tag{24a}$$

$$\{g_i(\boldsymbol{x}),Q_{jk}(\boldsymbol{x}')\}=-[\nabla_i Q_{jk}(\boldsymbol{x})]\,\delta(\boldsymbol{x}-\boldsymbol{x}')-\nabla_l\delta(\boldsymbol{x}-\boldsymbol{x}')\lambda_{jkil}(\boldsymbol{x}'), \tag{24b}$$

$$\{g_i(\boldsymbol{x}),g_j(\boldsymbol{x}')\}=-\nabla_i'[\,\delta(\boldsymbol{x}-\boldsymbol{x}')g_j(\boldsymbol{x}')]+\nabla_j\delta(\boldsymbol{x}-\boldsymbol{x}')g_i(\boldsymbol{x}'). \tag{24c}$$

From the kinetic part of the Hamiltonian, Eqs. (24a) and (24c) generate the divergence of the momentum flux tensor $g_i g_j/\rho$. From Eq. (24a) and the first term in Eq. (24b), the divergence of an elastic stress tensor including the pressure results. Finally, the second and third terms in Eq. (24b) produce an elastic coupling to the molecular field $\delta\mathcal{H}/\delta Q_{ij}$ of the liquid crystal.

C. Derivation of the central Poisson bracket

In this section, we present the derivation of the central Poisson bracket $\{Q_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\}$. We start with $\{R_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\}$, introduce the definition of the alignment tensor from Eq. (12), $R_{ij}(\boldsymbol{x})=R(\boldsymbol{x})Q_{ij}(\boldsymbol{x})$, apply the product rule for Poisson brackets, and finally arrive at

$$\{Q_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\}=\frac{1}{R(\boldsymbol{x})}\{R_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\} - \frac{Q_{ij}(\boldsymbol{x})}{R(\boldsymbol{x})}\{R(\boldsymbol{x}),g_k(\boldsymbol{x}')\}. \tag{25}$$

Calculating the single Poisson brackets, we employ

$$\frac{\partial \Delta x_i^{\beta\nu}}{\partial x_j^{\alpha\mu}}=\delta^{\alpha\beta}\delta_{ij}\left(\delta^{\mu\nu}-\frac{m^\mu}{m_0}\right), \tag{26}$$

$$\frac{\partial \delta(\boldsymbol{x}-\boldsymbol{x}^\beta)}{\partial x_j^{\alpha\mu}}=-\nabla_l\delta(\boldsymbol{x}-\boldsymbol{x}^\beta)\,\delta^{\alpha\beta}\frac{m^\mu}{m_0}, \tag{27}$$

where, in the course of the manipulations, m^μ/m_0 either sums up to one or gives a vanishing term due to the definition of the center of mass: $\Sigma_\mu m^\mu \Delta \boldsymbol{x}^{\alpha\mu}=0$. We also use a Taylor expansion of the δ function,

$$\delta(\boldsymbol{x}-\boldsymbol{x}'+\Delta\boldsymbol{x}^{\alpha\mu})=\delta(\boldsymbol{x}-\boldsymbol{x}')+\Delta x_l^{\alpha\mu}\nabla_l\delta(\boldsymbol{x}-\boldsymbol{x}') +O(\Delta x^2\nabla^2), \tag{28}$$

where $O(\cdots)$ means "order of." With these comments, the evaluation of the Poisson bracket for $\hat{R}_{ij}(\boldsymbol{x})$ is straightforward and the coarse-grained result reads

$$\begin{aligned}\{R_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\}={}&[\nabla_k R_{ij}(\boldsymbol{x})]\delta(\boldsymbol{x}-\boldsymbol{x}')+O(\Delta x^2\nabla^2)\\ &+[R_{ij}(\boldsymbol{x})\delta_{kl}+\tfrac{2}{3}R_{kl}(\boldsymbol{x})\delta_{ij}\\ &-R_{jl}(\boldsymbol{x})\delta_{ik}-R_{il}(\boldsymbol{x})\delta_{jk}]\nabla_l\delta(\boldsymbol{x}-\boldsymbol{x}')\\ &-R_t(\boldsymbol{x})(\delta_{ik}\delta_{jl}+\delta_{jk}\delta_{il}-\tfrac{2}{3}\delta_{ij}\delta_{kl})\\ &\times\nabla_l\delta(\boldsymbol{x}-\boldsymbol{x}'),\end{aligned} \tag{29}$$

where

$$R_t(\boldsymbol{x})=\frac{1}{6}\left[\sum_\alpha \operatorname{Tr}\boldsymbol{I}^\alpha\delta(\boldsymbol{x}-\boldsymbol{x}^\alpha)\right]_c. \tag{30}$$

As we discussed earlier, the components of the moment-of-inertia tensors $\boldsymbol{I}^\alpha$ relax in microscopic times to their molecule-independent value $\boldsymbol{I}$ with components $I_{||}$ and $I_\perp$. In this limit, we have

$$R_t(\boldsymbol{x})=\frac{I}{6\Delta I}R(\boldsymbol{x}). \tag{31}$$

To complete our calculation of $\{Q_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x})\}$, we need to evaluate $\{R(\boldsymbol{x}),g_k(\boldsymbol{x})\}$. To do so, we use the relation

$$\hat{R}_{ij}^\alpha\hat{R}_{ij}^\alpha=\tfrac{2}{3}(R^\alpha)^2 \tag{32}$$

to calculate

$$\{R^\alpha,p_k^{\alpha\mu}\}=\tfrac{3}{2}(R^\alpha)^{-1}\hat{R}_{ij}^\alpha\{\hat{R}_{ij}^\alpha,p_k^{\alpha\mu}\}. \tag{33}$$

Using this result and $R^\alpha=\Delta I^\alpha$, we obtain

$$\begin{aligned}\{\hat{R}(\boldsymbol{x}),\hat{g}_i(\boldsymbol{x}')\}={}&\nabla_i[\hat{R}(\boldsymbol{x})\delta(\boldsymbol{x}-\boldsymbol{x}')]+\mathrm{O}(\Delta x^2\nabla^2)\\ &-\sum_\alpha\frac{3}{\Delta I^\alpha}\left(\hat{R}_{ik}^\alpha\hat{R}_{kj}^\alpha+\frac{I^\alpha}{6}\hat{R}_{ij}^\alpha\right)\\ &\times\delta(\boldsymbol{x}-\boldsymbol{x}^\alpha)\nabla_j\delta(\boldsymbol{x}-\boldsymbol{x}').\end{aligned} \tag{34}$$

From Eq. (10), we find

$$\hat{R}_{ik}^\alpha\hat{R}_{kj}^\alpha=\tfrac{1}{3}\Delta I^\alpha\hat{R}_{ij}^\alpha+\tfrac{2}{9}(\Delta I^\alpha)^2\delta_{ij}. \tag{35}$$

So after coarse graining, Eq. (34), and replacing I^α by I and ΔI^α by ΔI, we obtain

$$\begin{aligned}\{R(\boldsymbol{x}),g_i(\boldsymbol{x}')\}={}&\nabla_i[R(\boldsymbol{x})]\delta(\boldsymbol{x}-\boldsymbol{x}')+O(\Delta x^2\nabla^2)\\ &-\left[\left(1+\frac{I}{2\Delta I}\right)R_{ij}(\boldsymbol{x})-\frac{1}{3}R(\boldsymbol{x})\delta_{ij}\right]\\ &\times\nabla_j\delta(\boldsymbol{x}-\boldsymbol{x}').\end{aligned} \tag{36}$$

Finally, combining Eqs. (29) and (36) in Eq. (25) leads to the Poisson bracket $\{Q_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\}$ of Eqs. (22) and (23).

IV. DERIVATION OF DIRECTOR DYNAMICS

In the nematic phase, the orientational order is uniaxial and the alignment tensor assumes the form

$$Q_{ij}(\boldsymbol{x})=[\hat{Q}_{ij}(\boldsymbol{x})]_c=S(\boldsymbol{x})[n_i(\boldsymbol{x})n_j(\boldsymbol{x})-\delta_{ij}/3], \tag{37}$$

where, on an average, the molecules point along the director $\boldsymbol{n}(\boldsymbol{x})$. Projecting $\boldsymbol{Q}$ on $n_i n_j$ in the definition $[\hat{R}_{ij}(\boldsymbol{x})]_c=R(\boldsymbol{x})Q_{ij}(\boldsymbol{x})$, and using $\hat{R}_{ij}^\alpha$ from Eq. (10) and $R(\boldsymbol{x})$ from Eqs. (18) gives the conventional Maier-Saupe order parameter

$$S(\boldsymbol{x})=\frac{m_0}{\rho(\boldsymbol{x})}\left[\sum_\alpha\frac{3}{2}\left(\cos^2\vartheta^\alpha-\frac{1}{3}\right)\delta(\boldsymbol{x}-\boldsymbol{x}^\alpha)\right]_c, \tag{38}$$

where ϑ^α is the angle of the principal axis of the molecule α relative to $\boldsymbol{n}(\boldsymbol{x})$ and m_0 is the molecular mass. Note that $[\cdots]_c$ means coarse graining over distances much larger than the molecular scale so that S is defined by averaging over many molecules. The prefactor m_0/ϱ has to appear, since S should not depend on the number density of the molecules.

A. Poisson brackets for the director

To derive the dynamic equations in the nematic phase with its constant $S(\boldsymbol{x})$, we need the Poisson brackets for the director. However, a direct microscopic definition of the director such that $\boldsymbol{n}(\boldsymbol{x})=[\hat{\boldsymbol{n}}(\boldsymbol{x})]_c$ does not exist. The director is only defined via the alignment tensor $\boldsymbol{Q}$ in Eq. (37). We therefore employ the macroscopic Poisson bracket $\{Q_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\}$, insert the uniaxial alignment tensor of Eq. (37), and apply the product rule for Poisson brackets:

$$\begin{aligned}\{Q_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\}=&[n_i(\boldsymbol{x})n_j(\boldsymbol{x})-\tfrac{1}{3}\,\delta_{ij}]\{S(\boldsymbol{x}),g_k(\boldsymbol{x}')\}\\&+S(\boldsymbol{x})n_i(\boldsymbol{x})\{n_j(\boldsymbol{x}),g_k(\boldsymbol{x}')\}\\&+S(\boldsymbol{x})n_j(\boldsymbol{x})\{n_i(\boldsymbol{x}),g_k(\boldsymbol{x}')\}.\end{aligned} \tag{39}$$

Taking the trace of this equation with respect to i,j and projecting it on $n_i(\boldsymbol{x})$ and $n_j(\boldsymbol{x})$, respectively, we obtain the relations

$$2S(\boldsymbol{x})n_i(\boldsymbol{x})\{n_i(\boldsymbol{x}),g_k(\boldsymbol{x}')\}=0, \tag{40a}$$

$$2\{S(\boldsymbol{x}),g_k(\boldsymbol{x}')\}=\{Q_{ij}(\boldsymbol{x}),g_k(\boldsymbol{x}')\}n_i(\boldsymbol{x})n_j(\boldsymbol{x}). \tag{40b}$$

Taking the dot product of Eq. (39) with $n_i(\boldsymbol{x})$ and using Eqs. (40) give the director-momentum Poisson bracket

$$\{n_i(\boldsymbol{x}),g_j(\boldsymbol{x}')\}=\frac{1}{S}\,\delta^T_{ik}\{Q_{kl}(\boldsymbol{x}),g_j(\boldsymbol{x}')\}n_l(\boldsymbol{x}), \tag{41}$$

where

$$\delta^T_{ij}=\delta_{ij}-n_in_j \tag{42}$$

is the projector on the space perpendicular to $\boldsymbol{n}(\boldsymbol{x})$. It has to appear since the derivative $\partial\boldsymbol{n}/\partial t$ has to be perpendicular to $\boldsymbol{n}$ itself due to $\boldsymbol{n}^2=1$. After insertion of Eq. (22) into Eq. (41), we arrive at the final expression

$$\{n_i(\boldsymbol{x}),g_j(\boldsymbol{x}')\}=[\nabla_jn_i(\boldsymbol{x})]\,\delta(\boldsymbol{x}-\boldsymbol{x}')-\lambda_{ijk}(\boldsymbol{x})\nabla_k\delta(\boldsymbol{x}-\boldsymbol{x}'), \tag{43}$$

with

$$\begin{aligned}\lambda_{ijk}&=\delta^T_{il}n_m\lambda_{lmjk}/S\\&=\tfrac{1}{2}\,(\delta^T_{ij}n_k-\delta^T_{ik}n_j)+\tfrac{1}{2}\,\lambda(\delta^T_{ij}n_k+\delta^T_{ik}n_j),\end{aligned} \tag{44}$$

where

$$\lambda=\frac{1}{3}\left(1+\frac{I}{\Delta I}\,\frac{1}{S}\right) \tag{45}$$

denotes a reactive coefficient. It depends on the Maier-Saupe order parameter and, in addition, on the molecular parameters I and ΔI. It agrees with Forster's result so the additional dynamic variable $R(\boldsymbol{x})$ does not affect its value [39]. In the case of needlelike molecules, $I/\Delta I=2$ and $\lambda=(1+2/S)/3$. If, in addition, all the molecules are completely aligned $(S=1)$, we obtain $\lambda=1$ and $\lambda_{ijk}=\delta^T_{ij}n_k$. This agrees with Volovik's result, who derived the Poisson bracket for the director on pure symmetry arguments [37], but it also demonstrates that the symmetry arguments are not sufficient for determining Poisson brackets in complex media. Finally, the Poisson bracket that enters the momentum balance reads

$$\begin{aligned}\{g_i(\boldsymbol{x}),n_j(\boldsymbol{x}')\}=&-[\nabla_in_j(\boldsymbol{x})]\,\delta(\boldsymbol{x}-\boldsymbol{x}')\\&-\nabla_k\delta(\boldsymbol{x}-\boldsymbol{x}')\lambda_{jik}(\boldsymbol{x}').\end{aligned} \tag{46}$$

B. Nondissipative velocities

To calculate the nondissipative velocities from Eq. (2), we need the Hamiltonian

$$\mathcal{H}=\int\frac{g^2(\boldsymbol{x})}{2\rho(\boldsymbol{x})}d^3x+F[\rho(\boldsymbol{x}),\boldsymbol{n}(\boldsymbol{x})]. \tag{47}$$

It consists of a kinetic part and a free energy $F[\rho(\boldsymbol{x}),\boldsymbol{n}(\boldsymbol{x})]=\int f(\rho,\boldsymbol{n},\boldsymbol{\nabla n})d^3x$, which is Frank's free energy plus a term purely depending on ρ.

In Sec. III B, we have already calculated the nondissipative velocity for the density of mass as $V^\rho=-\operatorname{div}\boldsymbol{g}(\boldsymbol{x})$. For the director, we obtain with Eq. (43),

$$V_i^{\boldsymbol{n}}=-\boldsymbol{v}(\boldsymbol{x})\cdot\nabla n_i(\boldsymbol{x})+\lambda_{ijk}(\boldsymbol{x})\nabla_kv_j(\boldsymbol{x}). \tag{48}$$

The first term on the right-hand side is the convective derivative of $\boldsymbol{n}$ and the second term introduces a reactive coupling to the deformation rate. Note that $\boldsymbol{n}\cdot\boldsymbol{V}^{\boldsymbol{n}}=0$, as it should be since $\boldsymbol{n}$ is a unit vector. The most complex term is the nondissipative velocity of the momentum density. It employs Eqs. (24a), (24c), and (46) to get

$$\begin{aligned}V_i^{\boldsymbol{g}}=&-\nabla_j\left[\frac{g_i(\boldsymbol{x})g_j(\boldsymbol{x})}{\rho(\boldsymbol{x})}\right]-\rho(\boldsymbol{x})\nabla_i\frac{\delta F}{\delta\rho(\boldsymbol{x})}+[\nabla_in_j(\boldsymbol{x})]\frac{\delta F}{\delta n_j(\boldsymbol{x})}\\&+\nabla_k\left[\lambda_{jik}(\boldsymbol{x})\frac{\delta F}{\delta n_j(\boldsymbol{x})}\right].\end{aligned} \tag{49}$$

The divergence of the momentum flux tensor originates from the kinetic part of the Hamiltonian; a surface term has been dropped since we are only interested in bulk properties. The fourth term introduces an elastic coupling to the molecular field $\delta F/\delta\boldsymbol{n}$. The second and the third term can be rewritten such (see the Appendix) that the pressure

$$p=\rho\frac{\partial f}{\partial\rho}-f \tag{50}$$

and the elastic stress tensor

$$\sigma^0_{ij}=-\frac{\partial f}{\partial\nabla_jn_k}\nabla_in_k, \tag{51}$$

known from the Ericksen-Leslie equations, appear. The nondissipative velocity finally reads

$$V_i^{\boldsymbol{g}}=-\nabla_j\left[\frac{g_i(\boldsymbol{x})g_j(\boldsymbol{x})}{\rho(\boldsymbol{x})}\right]-\nabla_ip+\nabla_j\sigma^0_{ij}+\nabla_k\left[\lambda_{jik}(\boldsymbol{x})\frac{\delta F}{\delta n_j(\boldsymbol{x})}\right]. \tag{52}$$

C. Dissipative terms

In this section, we collect the dissipative terms for the dynamic equations following the rules outlined in Sec. II. For the mass density ρ no such term appears since it obeys a conservation law.

The time derivative $\partial\boldsymbol{n}/\partial t$ couples to conjugate forces with a different sign under time reversal. A possible term involving $\delta\mathcal{H}/\delta\rho$ cannot occur since the dissipative tensor is a vector pointing along $\boldsymbol{n}$ due to symmetry, thus violating the requirement that $\partial\boldsymbol{n}/\partial t \perp \boldsymbol{n}$. A second dissipative term introduces a coupling to $\delta\mathcal{H}/\delta n_i = \delta F/\delta n_i$:

$$-\frac{1}{\gamma}\delta^T_{ij}\frac{\delta F}{\delta n_j}, \tag{53}$$

where γ is a rotational viscosity.

The time derivative of $\boldsymbol{g}$ can only couple to the velocity $v_i = \delta\mathcal{H}/\delta g_i$. Pure couplings to v_i are forbidden since they would break the Galilean invariance of the equations. Thus, we are led to $\nabla_j \eta_{ijkl}\nabla_k v_l = \nabla_j \sigma'_{ij}$ where we have introduced the viscous stress tensor σ'_{ij}. The tensor of viscosities η_{ijkl} possesses two permutation symmetries: (1) $\eta_{ijkl} = \eta_{jikl}$ since σ'_{ij} should be symmetric [44] and (2) $\eta_{ijkl} = \eta_{klij}$ since it is associated with the dissipative energy $\int \eta_{ijkl}\nabla_i v_j \nabla_k v_l d^3x$. Furthermore, it has to obey the local $D_{\infty h}$ symmetry of the nematic phase. It can therefore be written as a sum of terms that only contain δ_{ij} and n_i:

$$\begin{aligned}\eta_{ijkl} = {} & \overline{\alpha}_1 n_i n_j n_k n_l + \frac{\alpha_4}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\\ & + \frac{\overline{\alpha}_5 + \overline{\alpha}_6}{4}(n_i n_k \delta_{jl} + n_j n_k \delta_{il} + n_i n_l \delta_{jk} + n_j n_l \delta_{ik})\\ & + \rho_1 \delta_{ij}\delta_{kl} + \rho_2(\delta_{ij} n_k n_l + n_i n_j \delta_{kl}).\end{aligned} \tag{54}$$

The viscous stress tensor then takes the form [1]

$$\begin{aligned}\sigma'_{ij} = {} & \overline{\alpha}_1 n_i n_j n_k n_l A_{kl} + \alpha_4 A_{ij} + \frac{\overline{\alpha}_5 + \overline{\alpha}_6}{2}(n_i A_{jk} + n_j A_{ik}) n_k\\ & + \rho_1 \delta_{ij} A_{kk} + \rho_2(\delta_{ij} n_k n_l A_{kl} + n_i n_j A_{kk}),\end{aligned} \tag{55}$$

where the symmetrized velocity gradient $A_{ij} = (\boldsymbol{\nabla}_i v_j + \boldsymbol{\nabla}_j v_i)/2$ is also called strain rate tensor. The last two terms only appear in compressible fluids renormalize the pressure. Therefore, they do not occur in the Ericksen-Leslie equations. We will comment on the bars of some of the viscosities in the following section.

D. Final equations

Collecting the reactive and dissipative terms, we arrive at the final equations. We first obtain the conservation law for the density of mass:

$$\frac{\partial\rho}{\partial t} = -\boldsymbol{\nabla}\cdot\boldsymbol{g}. \tag{56}$$

The equation for the director reads

$$\frac{\partial n_i}{\partial t} = -\boldsymbol{v}\cdot\boldsymbol{\nabla} n_i + \lambda_{ijk}\nabla_k v_j - \frac{1}{\gamma}\delta^T_{ij}\frac{\delta F}{\delta n_j}, \tag{57}$$

where λ_{ijk} and the reactive coefficient λ are given in Eqs. (44) and (45). Note that $dn_i/dt = \partial n_i/\partial t + \boldsymbol{v}\cdot\boldsymbol{\nabla} n_i$ is the material derivative of n_i. If we write

$$\lambda_{ijk}\nabla_k v_j = \lambda\,\delta^T_{ij} n_k A_{jk} + \boldsymbol{\omega}\times\boldsymbol{n} \text{ with } \boldsymbol{\omega} = \tfrac{1}{2}\,\text{curl}\,\boldsymbol{v} \tag{58}$$

and introduce the rate of change of $\boldsymbol{n}$ relative to a vortex in the fluid,

$$\boldsymbol{N} = \frac{d\boldsymbol{n}}{dt} - \boldsymbol{\omega}\times\boldsymbol{n}, \tag{59}$$

we arrive at the Oseen equation well known from the Ericksen-Leslie theory:

$$\gamma_1 N_i + \gamma_2 \delta^T_{ij} A_{jk} n_k = -\delta^T_{ij}\frac{\delta F}{\delta n_j}, \tag{60}$$

where $\gamma_1 = \gamma$ and $\gamma_2 = -\lambda\gamma$. Note that the ratio of the two viscosities γ_2 and γ_1 is the reactive coeffcient λ which only depends on S and the two molecular parameters I and ΔI, as first derived by Forster in Ref. [39] and later by Kamien [35]. This coefficient determines the angle between the flow direction and the director in a shear field; a phenomenon called flow alignment.

Finally, for the momentum balance equation we obtain

$$\frac{\partial g_i}{\partial t} = -\nabla_j\left(\frac{g_i g_j}{\rho}\right) - \nabla_i p + \nabla_j \sigma^0_{ij} + \nabla_j\left(\lambda_{kij}\frac{\delta F}{\delta n_k}\right) + \nabla_j \sigma'_{ij}. \tag{61}$$

The first two terms correspond to the familiar material derivative $\rho dv_i/dt$. Our dynamic equation for the momentum density completely agrees with the momentum balance of Ericksen and Leslie. We have already identified the elastic stress tensor σ^0_{ij} in Eq. (51). The two terms in the second line give the complete viscous stress tensor σ^{EL}_{ij} of Ericksen and Leslie. To show this, we replace $\delta F/\delta n_k$ by the Oseen equation (60), use Eq. (55) for σ'_{ij}, and, after some manipulations, arrive at

$$\begin{aligned}\sigma^{EL}_{ij} &= \lambda_{kij}\frac{\delta F}{\delta n_k} + \sigma'_{ij}\\ &= \alpha_1 n_i n_j n_k n_l A_{kl} + \alpha_2 N_i n_j + \alpha_3 n_i N_j + \alpha_4 A_{ij} + \alpha_5 n_j n_k A_{ik}\\ &\quad + \alpha_6 n_i n_k A_{jk} + \rho_1 \delta_{ij} A_{kk} + \rho_2(\delta_{ij} n_k n_l A_{kl} + n_i n_j A_{kk}),\end{aligned} \tag{62}$$

where the Leslie viscosities α_i are related to our viscosities by

$$\alpha_1 = \overline{\alpha}_1 - \gamma\lambda^2, \tag{63a}$$

$$\alpha_2 = -\gamma(1+\lambda)/2, \tag{63b}$$

$$\alpha_3 = \gamma(1-\lambda)/2, \tag{63c}$$

$$\alpha_4 = \alpha_4, \tag{63d}$$

$$\alpha_5 = (\overline{\alpha}_5 + \overline{\alpha}_6)/2 + \gamma\lambda(1+\lambda)/2, \tag{63e}$$

$$\alpha_6 = (\overline{\alpha}_5 + \overline{\alpha}_6)/2 - \gamma\lambda(1-\lambda)/2. \tag{63f}$$

Notice that the two Onsager relations [1] and the Parodi relation [40] in the Ericksen-Leslie theory are automatically fulfilled in our approach:

$$\gamma_1 = \gamma = \alpha_3 - \alpha_2, \tag{64a}$$

$$\gamma_2 = -\lambda\gamma = \alpha_2 + \alpha_3, \tag{64b}$$

$$\alpha_2 + \alpha_3 = \alpha_6 - \alpha_5. \tag{64c}$$

We can therefore conclude that the formalism based on Poisson brackets completely reproduces the Ericksen-Leslie equations.

V. DYNAMIC EQUATIONS FOR THE ALIGNMENT TENSOR

Given the results of the preceding section, we are convinced that the formalism based on Poisson brackets is the right means to derive the dynamic equations for anisotropic fluids characterized by the alignment tensor $\boldsymbol{Q}$. We follow the systematic way of the formalism by collecting the reactive and dissipative terms first and then summarize and discuss the final equations.

A. Nondissipative velocities

The Hamiltonian has the following form:

$$\mathcal{H} = \int \frac{g^2(\boldsymbol{x})}{2\rho(\boldsymbol{x})} d^3x + F[\rho(\boldsymbol{x}), \boldsymbol{Q}(\boldsymbol{x})], \tag{65}$$

where $F[\rho(\boldsymbol{x}),\boldsymbol{Q}(\boldsymbol{x})] = \int f(\rho, \boldsymbol{Q}, \boldsymbol{\nabla Q}) d^3x$ stands for the Landau–de Gennes free energy plus a term purely depending on ρ.

The nondissipative velocity for the density of mass is clear. The reactive term for the alignment tensor reads

$$V_{ij}^{\boldsymbol{Q}} = -\boldsymbol{v}(\boldsymbol{x}) \cdot \boldsymbol{\nabla} Q_{ij}(\boldsymbol{x}) + \lambda_{ijkl}(\boldsymbol{x}) \nabla_l v_k(\boldsymbol{x}), \tag{66}$$

where $\lambda_{ijkl}(\boldsymbol{x})$ is defined in Eq. (23). Due to $Q_{ii}=0$ and $\lambda_{iikl}=0$, the velocity does not change the zero trace of the order parameter.

In the nondissipative velocity $V_i^{\boldsymbol{g}}$ of the momentum balance equation, we introduce, in full analogy to the director approach, the pressure $p = \rho \partial f / \partial \rho - f$ and the generalization of the Ericksen-Leslie elastic stress tensor

$$\sigma_{ij}^0 = -\frac{\partial f}{\partial \nabla_j Q_{kl}} \nabla_i Q_{kl}, \tag{67}$$

and finally arrive at

$$V_i^{\boldsymbol{g}} = -\nabla_j \left[\frac{g_i(\boldsymbol{x}) g_j(\boldsymbol{x})}{\rho(\boldsymbol{x})} \right] - \nabla_i p + \nabla_j \sigma_{ij}^0 + \nabla_j \left[\lambda_{klij}(\boldsymbol{x}) \frac{\delta F}{\delta Q_{kl}(\boldsymbol{x})} \right]. \tag{68}$$

B. Dissipative terms

The time derivative $\partial Q_{ij}/\partial t$ couples to $\delta F/\delta Q_{ij}$ via a fourth-rank tensor which should not alter the properties of $\boldsymbol{Q}$ being a symmetric tensor with zero trace. Furthermore, since we want to describe biaxial orientational ordering in the nematic phase, it has to obey the local symmetry of the alignment tensor given, in general, by the point group D_{2h}. To simplify our considerations, we only look for tensors which are invariant under $SO(3)$ and, therefore, arrive at the simplest dissipative term with the rotational viscosity γ:

$$-\frac{1}{\gamma}\left[\frac{1}{2}\left(\frac{\delta F}{\delta Q_{ij}} + \frac{\delta F}{\delta Q_{ji}}\right) - \frac{1}{3}\delta_{ij}\frac{\delta F}{\delta Q_{kk}}\right] =: -\frac{1}{\gamma}\left[\frac{\delta F}{\delta \boldsymbol{Q}}\right]_{ij}^{st}, \tag{69}$$

where the symbol $[\cdots]^{st}$ projects out the symmetric and traceless part of a second-rank tensor. In the general case, Eq. (69) would be replaced by $-\gamma_{ijkl}^{-1}[\delta F/\delta \boldsymbol{Q}]_{kl}^{st}$, where γ_{ijkl}^{-1} is a tensor function of $\boldsymbol{Q}$ that is symmetric under $ij \leftrightarrow kl$, $i \leftrightarrow j$, and $k \leftrightarrow l$ and traceless under contractions of both i and j and of k and l.

Following the time-reversal criterion, a coupling between $\partial Q_{ij}/\partial t$ and $\delta\mathcal{H}/\delta\rho$ is also possible. However, according to the Onsager principle such a term is not allowed since the related coupling of $\delta\mathcal{H}/\delta Q_{ij}$ to $\partial\rho/\partial t$ does not exist.

The dissipative term in the momentum balance equation is $\nabla_j \sigma'_{ij} = \nabla_j \eta_{ijkl} \nabla_k v_l$, where σ'_{ij} denotes the viscous stress tensor. The tensor of viscosities η_{ijkl} possesses the same permutation symmetries as in any isotropic system or in the director picture introduced before. However, now it has to reflect the local D_{2h} symmetry that gives rise to nine independent viscosities [45]. We will not formulate this tensor in its general form, rather we will write it as an expansion in $\boldsymbol{Q}$ up to the second order:

$$\begin{aligned}\eta_{ijkl} = {} & \eta_1 \delta_{ij}\delta_{kl} + \eta_2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \eta_3(\delta_{ij}Q_{kl} + Q_{ij}\delta_{kl}) \\ & + \eta_4(\delta_{ik}Q_{jl} + \delta_{jk}Q_{il} + \delta_{il}Q_{jk} + \delta_{jl}Q_{ik}) + \eta_5 Q_{ij}Q_{kl},\end{aligned} \tag{70}$$

which results in the following stress tensor:

$$\begin{aligned}\sigma'_{ij} = {} & \eta_1 \delta_{ij} A_{kk} + 2\eta_2 A_{ij} + \eta_3(\delta_{ij}Q_{kl}A_{kl} + Q_{ij}A_{kk}) \\ & + 2\eta_4(Q_{ik}A_{jk} + Q_{jk}A_{ik}) + \eta_5 Q_{ij}Q_{kl}A_{kl}.\end{aligned} \tag{71}$$

Of course, there are three further terms quadratic in $\boldsymbol{Q}$ that we left out in Eq. (70). The problem is that we have no clear criterion where to break up the expansion. We included one second-order term to be sure to reproduce all terms of the viscous stress tensor (55) in the director picture. Inserting the uniaxial $\boldsymbol{Q}$ into Eq. (71), we are able to relate the present viscosities to the one introduced in Eq. (54) or (55):

$$\bar{\alpha}_1 = \eta_5 S^2, \quad \alpha_4 = 2\eta_2 - \tfrac{2}{3}\eta_4 S, \quad \bar{\alpha}_5 + \bar{\alpha}_6 = 2\eta_4 S,$$

$$\rho_1 = \eta_1 - \tfrac{2}{3}\eta_3 S - \tfrac{1}{9}\eta_5 S^2, \quad \rho_2 = \eta_3 S - \tfrac{1}{3}\eta_5 S^2. \tag{72}$$

It is evident that the viscous stress tensor of Eq. (71) contains several shear viscosities which need to be worked out.

C. Final equations

In discussing our final equations, we will compare them to the set of equations derived by Olmstedt and Goldbart who followed the path outlined by de Gennes in Ref. [1] to derive the Ericksen-Leslie equations.

The density of mass obeys the mass-conservation law. The dynamic equation for the alignment tensor reads

$$\frac{\partial Q_{ij}}{\partial t} = -\boldsymbol{v}\cdot\boldsymbol{\nabla} Q_{ij} + \lambda_{ijkl}\nabla_l v_k - \frac{1}{\gamma}\left[\frac{\delta F}{\delta \mathbf{Q}}\right]^{st}_{ij}. \tag{73}$$

With $\lambda_{ijkl}(\boldsymbol{x})$ from Eq. (23), we obtain explicitly

$$\begin{aligned}\lambda_{ijkl}\nabla_l v_k = {} & Q_{il}W_{lj} - W_{il}Q_{lj} + \frac{1}{3}\frac{I}{\Delta I}[\boldsymbol{A}]^{st}_{ij} - \frac{2}{3}Q_{ij}A_{kk} \\ & + 2[\boldsymbol{QA}]^{st}_{ij} - \left(1+\frac{I}{\Delta I}\right)Q_{ij}Q_{kl}A_{kl},\end{aligned} \tag{74}$$

where $W_{ij}=(\nabla_i v_j - \nabla_j v_i)/2$ is the antisymmetric part of the velocity gradient. The commutator of $\boldsymbol{Q}$ and $\boldsymbol{W}$ on the right-hand side of Eq. (74) describes a rotation of $\boldsymbol{Q}$ due to a fluid vortex. With this in mind, we introduce, in the spirit of the Ericksen-Leslie equations, the new dynamic variable for the rate of change of the alignment tensor:

$$K_{ij} = \frac{dQ_{ij}}{dt} - (Q_{il}W_{lj} - W_{il}Q_{lj}) \tag{75}$$

and reformulate Eq. (73) as

$$\begin{aligned}K_{ij} = {} & -\frac{2}{3}Q_{ij}A_{kk} + \frac{1}{3}\frac{I}{\Delta I}[\boldsymbol{A}]^{st}_{ij} + 2[\boldsymbol{QA}]^{st}_{ij} \\ & - \left(1+\frac{I}{\Delta I}\right)Q_{ij}Q_{kl}A_{kl} - \frac{1}{\gamma}\left[\frac{\delta F}{\delta \mathbf{Q}}\right]^{st}_{ij}.\end{aligned} \tag{76}$$

This result is essentially the same as that obtained by Pleiner *et al.* [33], except that their result has additional terms quadratic in Q_{ij} and linear in A_{ij}. It is also very close to the result of Olmsted and Goldbart who derived their equation by a linear expansion of the dissipative flux ($\boldsymbol{K}$) into the generalized forces $[\boldsymbol{A}]^{st}_{ij}$ and $[\delta F/\delta \mathbf{Q}]^{st}$. The first term on the right-hand side vanishes for an incompressible fluid ($A_{kk}=0$) and, therefore, does not appear in the Olmsted-Goldbart approach. The second term has a reactive nature with a known coefficient ($I/3\Delta I$); it appears in the Olmsted-Goldbart treatment with an arbitrary coefficient ν_3. The third and fourth term do not appear in their treatment but, in their spirit, could be regarded as reactive terms of higher order in $\boldsymbol{Q}$. They necessarily appear in our approach with calculable coefficients. The last term has a dissipative nature in both approaches.

Finally, the momentum balance equation takes the form

$$\frac{\partial g_i}{\partial t} = -\nabla_j\left(\frac{g_i g_j}{\rho}\right) - \nabla_i p + \nabla_j \sigma^0_{ij} + \nabla_j\left(\lambda_{klij}\frac{\delta F}{\delta Q_{kl}}\right) + \nabla_j \sigma'_{ij}, \tag{77}$$

where the elastic (σ^0_{ij}) and viscous (σ'_{ij}) stress tensors are defined in Eqs. (67) and (71), respectively. Here, we also have a close resemblance with the result of Olmsted and Goldbart. The first line of Eq. (77) is identical to their expression. To investigate the second line, we write explicitly

$$\begin{aligned}\lambda_{klij}\frac{\delta F}{\delta Q_{kl}} = {} & -\frac{2}{3}\delta_{ij}Q_{kl}\left[\frac{\delta F}{\delta \mathbf{Q}}\right]^{st}_{kl} + 2Q_{jk}\left[\frac{\delta F}{\delta \mathbf{Q}}\right]^{st}_{ik} + \frac{1}{3}\frac{I}{\Delta I}\left[\frac{\delta F}{\delta \mathbf{Q}}\right]^{st}_{ij} \\ & - \left(1+\frac{I}{2\Delta I}\right)Q_{ij}Q_{kl}\left[\frac{\delta F}{\delta \mathbf{Q}}\right]^{st}_{kl}.\end{aligned} \tag{78}$$

The first term on the right-hand side renormalizes the pressure and, therefore, does not exist in the Olmsted-Goldbart approach. Furthermore, only the antisymmetric part of the second term appears in their paper. They had to introduce it in order to obtain the proper dissipation function

$$T\frac{dS}{dt} = \int\left\{\sigma'_{ij}A_{ij} + \frac{1}{\gamma}\left[\frac{\delta F}{\delta \mathbf{Q}}\right]^{st}_{ij}\left[\frac{\delta F}{\delta \mathbf{Q}}\right]^{st}_{ij}\right\}d^3x, \tag{79}$$

where $\gamma^{-1}[\delta F/\delta \mathbf{Q}]^{st}$ is the dissipative flux introduced in Eq. (69) in connection with the generalized force $[\delta F/\delta \mathbf{Q}]^{st}$. The third tensor on the right-hand side of Eq. (78) with its reactive coefficient $I/3\Delta I$ again corresponds to a dissipative term with the viscous coefficient ν_3 in the Olmsted-Goldbart approach. The fourth tensor, of second order in $\boldsymbol{Q}$, is new. Finally, Olmsted and Goldbart only introduced the isotropic part of the viscous stress tensor σ'_{ij} in Eq. (71), since they were close to the nematic-isotropic phase transition.

In conclusion, we find a remarkable agreement between our formalism and the approach by Olmsted and Goldbart. By identifying the reactive character of two of the terms, we are able to give a concrete value for the viscous coefficent ν_3 in the Olmsted-Goldbart paper in terms of the molecular parameters I and ΔI. Furthermore, we arrive quite naturally at additional terms with a reactive nature whose consequences need to be worked out.

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APPENDIX: PRESSURE AND ELASTIC STRESS TENSOR

To introduce the pressure p of Eq. (50) and the elastic stress tensor σ^0_{ij} of Eq. (51) in Eq. (49), we rewrite the second term on the left-hand side as

$$-\rho\nabla_i \frac{\delta F}{\delta\rho} = -\nabla_i(f+p) + (\nabla_i\rho)\frac{\partial}{\partial\rho} f \tag{A1}$$

and the third term as

$$(\nabla_i n_j)\frac{\delta F}{\delta n_j} = (\nabla_i n_j)\left(\frac{\partial f}{\partial n_j} - \nabla_k \frac{\partial f}{\partial \nabla_k n_j}\right). \tag{A2}$$

The sum of both terms together with

$$\nabla_i f = \frac{\partial f}{\partial\rho}\nabla_i\rho + \frac{\partial f}{\partial n_j}\nabla_i n_j + \frac{\partial f}{\partial \nabla_k n_j}\nabla_k(\nabla_i n_j) \tag{A3}$$

gives p and σ_{ij}^0.

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