Poisson bracket approach to the dynamics of nematic liquid crystals: The role of spin angular momentum

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(Received 9 June 2005; published 17 November 2005)

Nematic liquid crystals are well modeled as a fluid of rigid rods. Starting from this model, we use a Poisson-bracket formalism to derive the equations governing the dynamics of nematic liquid crystals. We treat the spin angular momentum density arising from the rotation of constituent molecules about their centers of mass as an independent field and derive equations for it, the mass density, the momentum density, and the nematic director. Our equations reduce to the original Leslie-Ericksen equations, including the inertial director term that is neglected in the hydrodynamic limit, only when the moment of inertia for angular momentum parallel to the director vanishes and when a dissipative coefficient favoring locking of the angular frequencies of director rotation and spin angular momentum diverges. Our equations reduce to the equations of nematohydrodynamics in the hydrodynamic limit but with dissipative coefficients that depend on the coefficient that must diverge to produce the Leslie-Ericksen equations.

DOI: 10.1103/PhysRevE.72.051714 PACS number(s): 61.30.−v, 47.50.+d

I. INTRODUCTION

The Leslie-Ericksen (LE) equations [1] for the dynamics of nematic liquid crystals have been a bulwark of liquid crystal science since they were first derived over 40 years ago. For a historical account of their derivation see Ref. [2]. They indisputably provide a correct theoretical description of the almost limitless variety of dynamical phenomena that nematic liquid crystals can exhibit, from simple shear flow to hydrodynamic instabilities to complex switching in display cells.

The equations originally derived by Leslie and Ericksen are not completely hydrodynamical. They contain an inertial term in the equation for the director, **n**, specifying the direction of molecular alignment, that leads to modes that decay in microscopic times. When this term is ignored, the resulting equations are purely hydrodynamical with mode frequencies that all vanish with vanishing wave number. Subsequent treatments [3,4] of the dynamics of nematics produced purely hydrodynamical equations from the outset. To our knowledge, all of the many experimental verifications of the validity of the LE equations probe only the hydrodynamic limit; they do not test the existence of or the form of the nonhydrodynamic part of the original LE equations.

The LE equations and purely hydrodynamic treatments of nematodynamics differ most profoundly in their treatment of kinetic energy. In the hydrodynamic theories [3,4], the momentum density **g** and its related velocity field **v** measure the momentum of all mass points in the medium including those along the full length of rigid mesogens. This momentum is a conserved quantity and is necessarily hydrodynamic. The energy density is $g^2/(2\rho)$, where ρ is the mass density. Since **g** is the total momentum density, it contains all information about angular momentum, and it is not necessary to introduce additional variables to describe what we will call the spin angular momentum associated with rotation of constituent rigid molecules about their centers of mass [3,5]. The other variables that appear in the hydrodynamic treatment are the conserved mass density and the Frank director **n**. In the LE treatment, there are two contributions to the kinetic energy, a translational part $g^2/(2\rho)$ and a rotational part, $\mathcal{I}_\perp(\mathbf{n}\times\dot{\mathbf{n}})^2/2$, where $\mathcal{I}_\perp$ is a moment of inertia density, arising from motion of the director. The interpretation of this decomposition [1] of the kinetic energy is that **g** is now the center-of-mass momentum density, which is a conserved variable, and that the director contribution to the kinetic energy arises from the spin angular momentum. There are now two contributions to the angular momentum, the spin angular momentum and that arising from center-of-mass motion. Neither contribution is individually conserved, but their sum is. In the LE treatment, the equation for the director is basically an equation for the spin angular momentum, which is neither a conserved nor a hydrodynamical variable and which, therefore, has nonhydrodynamic decays in it.

Though the LE equations are internally consistent and reduce to the correct hydrodynamical form when the inertial term is ignored, they in fact do not provide a correct description of spin angular momentum. Spin angular momentum is an independent dynamical variable that is not locked to the director, though in steady state situations it does relax to a value determined by the local director and its rotation rate. The spin kinetic energy is determined by the spin angular momentum and not by the dynamics of the director. In this paper, we describe the dynamics of nematics in terms of their nonconserved spin angular momentum density, their conserved mass density and center-of-mass momentum density, and their director. For simplicity, we consider isothermal processes only, and we ignore the equations of energy conservation. We use the Poisson-bracket approach [6–11,13–15] to derive the equations of motion for these variables. The hydrodynamical limit of our equations is identical to that of the LE equations but with a slightly different interpretation of some dissipative coefficients. Our equations also reduce to the full LE equations when an appropriate viscosity diverges

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and spin angular momentum parallel to the director is ignored. Previous investigations [13,16] have noted that spin angular momentum should be treated as an independent variable and argued that it will decay in microscopic times to a value determined by the director. They do not, however, provide a detailed prescription for how this decay occurs or the conditions under which the original LE equation can be retrieved. Finally, our equations reduce to the hydrodynamical equations for rigid rotors on a lattice [10] when coupling to center-of-mass motion is turned off.

Since the derivation of our results is at times algebraically tedious, we review our main results in Sec. II. We present first the dynamical equations that result from our analysis and show how they reduce to the LE equations and to true hydrodynamical equations in the appropriate limit. In Sec. III we briefly summarize the Poisson-bracket formalism. In Sec. IV we introduce the fluid of rigid rods and the relevant dynamic variables and their Poisson brackets. Finally, in Sec. V, we derive the equations of nematodynamics with spin angular momentum.

II. REVIEW OF RESULTS

We model our nematic as a collection of uniaxial rigid rods. The coarse-grained variables describing this system are the mass density ρ, the center-of-mass momentum density $\mathbf{g}=\rho\mathbf{v}$, the spin angular momentum density $\mathbf{l}$, and the nematic director $\mathbf{n}$. The angular momentum density $\mathbf{l}=\mathcal{I}\boldsymbol{\Omega}$ can be expressed in terms of a moment-of-inertia density $\mathcal{I}_{ij}=\mathcal{I}_\parallel n_i n_j+\mathcal{I}_\perp(\delta_{ij}-n_i n_j)$ and an angular frequency $\boldsymbol{\Omega}$. The full equations for all of these variables are

$$\frac{d\rho}{dt}+\rho\boldsymbol{\nabla}\cdot\mathbf{v}=0, \tag{2.1}$$

$$\frac{\partial g_i}{\partial t}=-\nabla_j\left(\frac{g_i g_j}{\rho}\right)-\nabla_i p+\nabla_j\sigma_{ij}, \tag{2.2}$$

$$\frac{d\mathbf{n}}{dt}=\boldsymbol{\Omega}\times\mathbf{n}+\frac{1}{\gamma}[\mathbf{h}+\Delta\mathcal{I}\Omega_\parallel\boldsymbol{\Omega}_\perp], \tag{2.3}$$

$$\mathcal{I}_\perp\left(\frac{d\boldsymbol{\Omega}_\perp}{dt}\right)_\perp+\mathcal{I}_\parallel\Omega_\parallel\frac{d\mathbf{n}}{dt}=\mathbf{n}\times\mathbf{h}-\Gamma_\perp^\Omega(\boldsymbol{\Omega}_\perp-\boldsymbol{\omega}_\perp)-\Gamma^A(\mathbf{An})\times\mathbf{n}, \tag{2.4}$$

$$\mathcal{I}_\parallel\frac{d\Omega_\parallel}{dt}-\frac{\mathcal{I}_\perp}{\gamma}(\boldsymbol{\Omega}_\perp\cdot\mathbf{h}+\Delta\mathcal{I}\Omega_\parallel\Omega_\perp^2)=-\Gamma_\parallel^\Omega(\Omega_\parallel-\omega_\parallel), \tag{2.5}$$

where $\Delta\mathcal{I}=\mathcal{I}_\parallel-\mathcal{I}_\perp$, $\mathbf{h}$ is the molecular field with components $h_i=-(\delta_{ij}-n_i n_j)\delta F/\delta n_i$, where F is the free energy, p is the pressure, σ_{ij} is the dissipative and director part of the stress tensor, $\mathbf{A}$ is the symmetrized strain rate tensor with components $(\partial_i v_j+\partial_j v_i)/2$, and $\boldsymbol{\omega}=(\boldsymbol{\nabla}\times\mathbf{v})/2$ is half the local vorticity. In these equations, $dA/dt=\partial A/\partial t+\mathbf{v}\cdot\boldsymbol{\nabla}A$ is the total derivative of any field A, $c_\parallel=\mathbf{n}\cdot\mathbf{c}$ is the component of any vector $\mathbf{c}$ along $\mathbf{n}$ and $\mathbf{c}_\perp=\mathbf{n}\times(\mathbf{c}\times\mathbf{n})$ its component perpendicular to $\mathbf{n}$, and $\mathbf{An}$ is the product of a matrix with a vector with components $A_{ij}n_j$. The stress tensor σ_{ij} can be decomposed into elastic, viscous symmetric, and viscous antisymmetric parts,

$$\sigma_{ij}=\sigma_{ij}^E+\sigma_{ij}^{S\prime}+\sigma_{ij}^{A\prime}, \tag{2.6}$$

where

$$\sigma_{ij}^E=-\frac{\partial f}{\partial\nabla_j n_k}\nabla_i n_k, \tag{2.7}$$

$$\sigma_{ij}^{S\prime}=\alpha_{ijkl}A_{kl}+\tfrac{1}{2}\Gamma^A(\varepsilon_{ilk}n_j n_l+\varepsilon_{jlk}n_i n_l)(\Omega_k-\omega_k), \tag{2.8}$$

$$\sigma_{ij}^{A\prime}=\tfrac{1}{2}\varepsilon_{ijk}\Gamma_{kl}^\Omega(\Omega_l-\omega_l)+\tfrac{1}{2}\Gamma^A(n_j A_{\mathrm{in}}n_n-n_i A_{jn}n_n). \tag{2.9}$$

with $\Gamma_{kl}^\Omega=\Gamma_\parallel^\Omega n_i n_j+\Gamma_\perp^\Omega(\delta_{ij}-n_i n_j)$ and α_{ijkl} a fourth-rank tensor of uniaxial symmetry given explicitly in Eq. (5.22).

Equations (2.1)–(2.9) provide a complete description of the dynamics of nematics. Equations (2.1) and (2.2) are the familiar conservation laws for mass and momentum. Equation (2.3) is the equation of motion for the director. It is similar to that of the full hydrodynamical theory derived by the Harvard group [3] except that the reactive term $\boldsymbol{\Omega}\times\mathbf{n}$ depends only on the spin frequency $\boldsymbol{\Omega}$ and not on $\mathbf{A}$ and $\boldsymbol{\omega}$. If $\gamma^{-1}=0$, the director simply rotates like a rigid-body axis perpendicular to the angular spin $\boldsymbol{\Omega}$. When γ^{-1} is nonzero, director motion decays to $\boldsymbol{\Omega}\times\mathbf{n}$ in a time of order $K/(\gamma q^2)$ where K is a Frank elastic constant and q is the spatial wave number of director distortions. Equations (2.4) and (2.5) are the torque equations for spin angular momentum. The spin frequency $\Omega_\parallel$ parallel to the director, described by Eq. (2.5), is a nonhydrodynamic variable that decays in microscopic times to $\omega_\parallel$ plus nonlinear terms. It cannot be ignored except in the hydrodynamic limit or in the limit in which only the component of spin angular momentum perpendicular to the director survives, i.e., when $\mathcal{I}_\parallel=0$, which occurs in the limit of perfect nematic order in a system composed of infinitely thin rods. Equation (2.5) contains a nonlinear term proportional to $\Omega_\parallel\boldsymbol{\Omega}_\perp$ that has physical significance. As reviewed in Appendix A, it causes the axis with the highest moment of inertia to align along the direction of the angular momentum in rigid body motion with conserved angular momentum but not energy. The right-hand sides of Eqs. (2.4) and (2.5) are the time rate of change, $d\mathbf{l}/dt$, of the spin angular momentum projected, respectively, along directions perpendicular and parallel to $\mathbf{n}$. In the absence of dissipation, $d\mathbf{l}/dt$ is simply the torque density $\mathbf{n}\times\mathbf{h}$ appearing in Eq. (2.4). Rigid-body rotation in which $\boldsymbol{\Omega}=\boldsymbol{\omega}$ and $\mathbf{A}=\mathbf{0}$ is a stationary state in which $d\mathbf{l}/dt=\mathbf{0}$. If $\boldsymbol{\Omega}\neq\boldsymbol{\omega}$, dissipative torques, given by the $\Gamma_\perp^\Omega$ and $\Gamma_\parallel^\Omega$ terms in Eqs. (2.4) and (2.5), drive $\boldsymbol{\Omega}$ towards $\boldsymbol{\omega}$. Spin angular momentum is also reoriented via the Γ^A term in Eq. (2.4) by the symmetric strain rate $\mathbf{A}$ when it is nonzero. The stress tensor contains a couple of terms not found in isotropic fluids. The antisymmetric parts of the stress tensor proportional to Γ_A and Γ_{ij}^Ω are dictated by the requirement that the total spin and center-of-mass angular momentum is conserved (see Appendix B). The Γ^A contribution to the symmetric part of the dissipative srress tensor $\sigma_{ij}^{S\prime}$ is a consequence of an Onsager relation.

When $\Gamma_{\parallel}^{\Omega}$, $\Gamma_{\perp}^{\Omega}$, and Γ^{A} are zero, spin angular momentum is conserved, and additional diffusive dissipative terms proportional to $\nabla^2\mathbf{\Omega}$ must be added to Eqs. (2.4) and (2.5) for a complete description. In this limit, Eq. (2.3) along with Eqs. (2.4) and (2.5) provide a hydrodynamical description of rigid rotors on a rigid lattice with frictionless bearings, which exhibit spin-wave excitations with a frequency dispersion $\omega \sim q$ with q the wave number [10].

We can now consider under what conditions our equations reduce to the original LE equations and how the hydrodynamical limit is obtained. We begin with obtaining the LE equations. To approach the LE limit, we use Eq. (2.3) to replace $\mathbf{\Omega}\times\mathbf{n}$ by $(d\mathbf{n}/dt)-\gamma^{-1}\mathbf{h}^T$, where $\mathbf{h}^T=\mathbf{h}+\Delta\mathcal{I}\Omega_{\parallel}\mathbf{\Omega}_{\perp}$. This converts Eq. (2.4) to

$$\mathcal{I}_{\perp}\mathbf{n}\times\left(\frac{d^2\mathbf{n}}{dt^2}-\frac{1}{\gamma}\frac{d\mathbf{h}^T}{dt}\right)+\mathcal{I}_{\parallel}\Omega_{\parallel}\frac{d\mathbf{n}}{dt}-\frac{\Gamma_{\perp}^{\Omega}\Delta\mathcal{I}}{\gamma}\Omega_{\parallel}\mathbf{n}\times\mathbf{\Omega}$$
$$=\alpha\mathbf{n}\times(\mathbf{h}-\gamma_1\mathbf{N}-\gamma_2\mathbf{A}\mathbf{n}), \tag{2.10}$$

where we introduced

$$\mathbf{N}=\frac{d\mathbf{n}}{dt}-\boldsymbol{\omega}\times\mathbf{n} \tag{2.11}$$

and

$$\alpha=1+\frac{\Gamma_{\perp}^{\Omega}}{\gamma},\quad \frac{1}{\gamma_1}=\frac{1}{\gamma}+\frac{1}{\Gamma_{\perp}^{\Omega}},\quad \gamma_2=-\frac{\Gamma^{A}}{\Gamma_{\perp}^{\Omega}}\gamma_1\equiv-\lambda\gamma_1. \tag{2.12}$$

Equation (2.10) reduces identically to the original LE equation [1] for the director with left-hand side equal to $\mathcal{I}_{\perp}\mathbf{n}\times d^2\mathbf{n}/dt^2$, $\alpha=1$ and $\gamma_1=\Gamma_{\perp}^{\Omega}$, when $\gamma\to\infty$ and $\mathcal{I}_{\parallel}=0$. The first condition, $\gamma\to\infty$, constrains $d\mathbf{n}/dt$ to be $\mathbf{\Omega}\times\mathbf{n}$. The second condition, $\mathcal{I}_{\parallel}=0$, is equivalent to there being no rotational kinetic energy associated with $\Omega_{\parallel}$ and is one that is tacitly assumed in the original LE approach for which the spin kinetic energy density is $\mathcal{I}_{\perp}(\mathbf{n}\times\dot{\mathbf{n}})^2/2$. We will show that $\mathcal{I}_{\parallel}$ vanishes for rigid rods when the Maier-Saupe order parameter S equals one, i.e., only when there is perfect order. If nematogens are modeled by more complex rigid structures than thin rods, $I_{\parallel}$ would be nonzero even for $S=1$. In the LE limit, Eq. (2.5) for $\Omega_{\parallel}$ implies that $\Omega_{\parallel}=\omega_{\parallel}$. Together with $\mathbf{\Omega}_{\perp}-\boldsymbol{\omega}_{\perp}=\mathbf{n}\times\mathbf{N}$, which follows from $d\mathbf{n}/dt=\mathbf{\Omega}\times\mathbf{n}$ and the definition for $\mathbf{N}$, the equations for the stress tensor [Eqs. (2.8) and (2.9)] assume exactly the form of the LE stress tensor. Thus to reiterate, the LE equations describe a nematic liquid crystal in which the director is forced to follow $\mathbf{\Omega}\times\mathbf{n}$ and the moment of inertial density parallel to the director is zero. Neither of these conditions apply in general.

To obtain the hydrodynamic limit, we discard all terms that are higher order in time and space derivatives than the dominant ones. This means that we can ignore the $d\Omega_{\parallel}/dt$ and the nonlinear terms in Eq. (2.5) relative to $\Omega_{\parallel}-\omega_{\parallel}$. Thus to hydrodynamic order, we can set $\Omega_{\parallel}=\omega_{\parallel}$. This procedure effectively removes $\Omega_{\parallel}$ from the problem. Similarly, we can ignore the $\Omega_{\parallel}$ term in the director equation [Eq. (2.3)] and all of the terms on the left-hand side of Eq. (2.10). The latter condition gives the familiar LE equation, $\mathbf{h}=\gamma_1\mathbf{N}+\gamma_2(\mathbf{A}\mathbf{n})_{\perp}$, for the director in which the inertial term is neglected. To obtain the hydrodynamic limit for the stress tensor, we use the hydrodynamic limit of Eqs. (2.3) and (2.10) and the relations in Eq. (2.12) to set

$$(\mathbf{\Omega}-\boldsymbol{\omega})\times\mathbf{n}=\frac{\gamma_1}{\Gamma_{\perp}^{\Omega}}\mathbf{N}-\frac{\gamma_2}{\gamma}(\mathbf{A}\mathbf{n})_{\perp} \tag{2.13}$$

and obtain

$$\sigma_{ij}^{A\prime}=\frac{1}{2}\gamma_1(n_iN_j-n_jN_i)+\frac{1}{2}\gamma_2[n_i(\mathbf{A}\mathbf{n})_{\perp j}-n_j(\mathbf{A}\mathbf{n})_{\perp i}], \tag{2.14}$$

$$\sigma_{ij}^{S\prime}=\alpha_{ijkl}A_{kl}+\frac{1}{2}\gamma_2(n_iN_j+n_jN_i)$$
$$-\frac{1}{2}\frac{(\Gamma^{A})^2}{\gamma+\Gamma_{\perp}^{\Omega}}[n_i(\mathbf{A}\mathbf{n})_{\perp j}+n_j(\mathbf{A}\mathbf{n})_{\perp i}]. \tag{2.15}$$

This is precisely the LE stress tensor in the hydrodynamic limit.

An important consequence of this analysis that treats angular momentum as an independent variable is that it demonstrates that two distinct effects contribute to the viscosity γ_1, the director damping measured by γ and the rotational friction measured by $\Gamma_{\perp}^{\Omega}$. γ_1 is the parallel combination of γ and $\Gamma_{\perp}^{\Omega}$ [see Eq. (2.12)].

In Ref. [11] we derived dynamical equations for the full nematic order parameter $\mathbf{Q}$, also called alignment tensor, using the Poisson-bracket formalism without, however, introducing the spin angular momentum density as a separate dynamic variable. With the approach presented in the following, we could also derive dynamic equations for $\mathbf{Q}$ and then by projection on the uniaxial part of $\mathbf{Q}$ arrive at an additional dynamic equation for the scalar order parameter. A similar consideration following Eqs. (2.10)–(2.12) should then lead to the extended LE equations of Ref. [12], where a variable S is taken into account. The field S is a nonhydrodynamic variable that relaxes in microscopic times. It does not, however, contribute to dissipative coefficients in the hydrodynamic limit as the spin angular momentum, which also has a rapidly decaying nonhydrodynamic component, does [see Eq. (2.12)]. We will, therefore, not treat S (or the biaxial part of $\mathbf{Q}$) in what follows.

In the remainder of the paper we give a detailed account of how the set of equations discussed in this section were derived. We start with a short review of the Poisson-bracket formalism.

III. GENERAL FORMALISM

In this section we collect the important formulas of the Poisson-bracket formalism. A more thorough explanation including original references can be found in our previous paper [11] and in Ref. [10].

We consider a systems whose microscopic dynamics is determined by canonically conjugate variables $\mathbf{q}^{\alpha}$ and $\boldsymbol{\pi}^{\alpha}$ for each particle α and a microscopic Hamiltonian $\hat{\mathcal{H}}(\{\mathbf{q}^{\alpha}\},\{\boldsymbol{\pi}^{\alpha}\})$. Rotational degrees of freedom may be in-

cluded in the coordinates $\mathbf{q}^\alpha$ and momenta $\boldsymbol{\pi}^\alpha$. We are interested in the slow dynamics of of a set of macroscopic field variables $\Phi_\mu(\mathbf{x},t)$ $(\mu=1,2,\ldots)$ obtained from microscopic fields $\hat{\Phi}_\mu(\mathbf{x},\{\mathbf{q}^\alpha\},\{\boldsymbol{\pi}^\alpha\})$ by coarse-graining over spatial fluctuations on the microscopic level; $\Phi_\mu(\mathbf{x},t)=[\hat{\Phi}_\mu(\mathbf{x},\{\mathbf{q}^\alpha\},\{\boldsymbol{\pi}^\alpha\})]_c$, where the symbol $[\cdots]_c$ specifies the coarse-grained averages. The statistical mechanics of the macroscopic fields $\Phi_\mu(\mathbf{x},t)$ is determined by the coarse-grained Hamiltonian $\mathcal{H}[\{\Phi_\mu\}]$.

Following the theory of kinetic or stochastic equations, the macroscopic variables evolve according to

$$\frac{\partial\Phi_\mu(\mathbf{x},t)}{\partial t}=V_\mu(\mathbf{x})-\Gamma_{\mu\nu}\frac{\delta\mathcal{H}}{\delta\Phi_\nu(\mathbf{x})}, \tag{3.1}$$

where we disregard any noise. The reactive term $V_\mu(\mathbf{x})$, also called the nondissipative or streaming velocity, is expressed with the help of Poisson brackets as

$$V_\mu(\mathbf{x})=-\int d^3x'\mathcal{P}_{\mu\nu}(\mathbf{x},\mathbf{x}')\frac{\delta\mathcal{H}}{\delta\Phi_\nu(\mathbf{x}')}, \tag{3.2}$$

where Einstein's convention on repeated indices is understood and

$$\mathcal{P}_{\mu\nu}(\mathbf{x},\mathbf{x}')=\{\Phi_\mu(\mathbf{x}),\Phi_\nu(\mathbf{x}')\}=-\mathcal{P}_{\nu\mu}(\mathbf{x}',\mathbf{x}) \tag{3.3}$$

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

$$\{\Phi_\mu(\mathbf{x}),\Phi_\nu(\mathbf{x}')\}=[\{\hat{\Phi}_\mu(\mathbf{x}),\hat{\Phi}_\nu(\mathbf{x}')\}]_c, \tag{3.4}$$

where [17]

$$\{\hat{\Phi}_\mu(\mathbf{x}),\hat{\Phi}_\nu(\mathbf{x}')\}=\sum_{\alpha i}\frac{\partial\hat{\Phi}_\mu(\mathbf{x})}{\partial\pi_i^\alpha}\frac{\partial\hat{\Phi}_\nu(\mathbf{x}')}{\partial q_i^\alpha}-\frac{\partial\hat{\Phi}_\mu(\mathbf{x})}{\partial q_i^\alpha}\frac{\partial\hat{\Phi}_\nu(\mathbf{x}')}{\partial\pi_i^\alpha}. \tag{3.5}$$

Since we only employ a restricted number of macroscopic variables, all the "neglected" microscopic degrees of freedom give rise to the dissipative term in the kinetic equation (3.1) that is proportional to the generalized force $\delta\mathcal{H}/\delta\Phi_\nu(\mathbf{x})$, which together with $\Phi_\nu(\mathbf{x})$ forms a pair of conjugate variables. The dissipative tensor $\Gamma_{\mu\nu}$ may depend on the fields Φ_μ and it may also contain terms proportional to $-\boldsymbol{\nabla}^2$. It is determined by three principles. First, the dissipative contributions to the equation for $\partial\Phi_\mu/\partial t$ must have the same sign under time reversal as Φ_μ (and thus the opposite sign to that of $\partial\Phi_\mu/\partial t$). Second, $\Gamma_{\mu\nu}$ must reflect the local point group symmmetry of the dynamical system, and third, it must be a symmetric tensor at zero magnetic field to obey the Onsager principle [18]. In the following, the last point will be important in identifying the proper dissipative terms in the momentum balance.

IV. POISSON BRACKETS FOR NEMATIC LIQUID CRYSTALS

A. Model molecule and dynamic variables

We model our system as a fluid of uniaxial rigid rods of length a and mass m. We describe the position of molecule α by its center-of-mass coordinate $\mathbf{x}^\alpha$ and its orientation by the unit vector $\hat{\boldsymbol{\nu}}^\alpha$. The center-of-mass momentum is $\mathbf{p}^\alpha=m\mathbf{v}^\alpha=m\dot{\mathbf{x}}^\alpha$ where the dot means total time derivative. With the help of the molecular order-parameter tensor Q^α with components

$$Q_{ij}^\alpha=\hat{\nu}_i^\alpha\hat{\nu}_j^\alpha-\tfrac{1}{3}\delta_{ij}, \tag{4.1}$$

the molecular moment-of-inertia tensor (relative to the center of mass) reads

$$I_{ij}^\alpha=I_\parallel\hat{\nu}_i^\alpha\hat{\nu}_j^\alpha+I_\perp(\delta_{ij}-\hat{\nu}_i^\alpha\hat{\nu}_j^\alpha)=\Delta IQ_{ij}^\alpha+\left(\tfrac{2}{3}I_\perp+\tfrac{1}{3}I_\parallel\right)\delta_{ij}, \tag{4.2}$$

where $I_\perp$ and $I_\parallel<I_\perp$ are the moments of inertia for rotations about axes perpendicular and parallel to $\hat{\boldsymbol{\nu}}^\alpha$, respectively, and $\Delta I=I_\parallel-I_\perp$. Note that $I_\parallel=0$, and $\Delta I=-I_\perp$ in the limit of infinitely thin rods. The tensor $\mathbf{I}^\alpha$ relates the spin angular momentum of a molecule, $\mathbf{l}^\alpha$, to its angular velocity $\boldsymbol{\Omega}^\alpha$,

$$l_i^\alpha=I_{ij}^\alpha\Omega_j^\alpha. \tag{4.3}$$

Note that $\mathbf{l}^\alpha$ is always perpendicular to $\hat{\boldsymbol{\nu}}^\alpha$ as it should be for an infinitely thin rod.

The microscopic Poisson bracket in Eq. (3.5) consists of a spatial and an angular part. The spatial contribution arises from the coordinate $\mathbf{x}^\alpha$ and its conjugate momentum $\mathbf{p}^\alpha$, which fulfill the canonical Poisson bracket [17],

$$\{p_i^\alpha,x_j^\beta\}=\delta^{\alpha\beta}\delta_{ij}, \tag{4.4}$$

where $\delta^{\alpha\beta}$ and δ_{ij} are Kronecker symbols. However, the unit vector $\hat{\boldsymbol{\nu}}^\alpha$ and the angular momentum $\mathbf{l}^\alpha$ are not canonically conjugate to each other since their Poisson bracket [17]

$$\{l_i^\alpha,\hat{\nu}_j^\beta\}=-\delta^{\alpha\beta}\varepsilon_{ijk}\hat{\nu}_k^\beta, \tag{4.5}$$

does not have the canonical form (ε_{ijk} denotes the Levi-Civita symbol). We could now introduce appropriate pairs of conjugate angular coordinates and momenta via a microscopic Legendre function. Instead, we follow an alternative route. It turns out that, in the following, Eq. (4.5) and the additional formula

$$\{l_i^\alpha,l_j^\beta\}=-\delta^{\alpha\beta}\varepsilon_{ijk}l_k^\beta \tag{4.6}$$

are sufficient for calculating the angular part of Poisson bracket (3.5). All other Poisson brackets, in particular the ones between the spatial and angular variables, are zero. The Poisson brackets in Eqs. (4.5) and (4.6) are a consequence of the fact that l_i^α is the generator of rotations about the molecular center of mass [13]. They can, or course, be derived from a Hamiltonian formalism for rigid rods in which the rotational kinetic energy depends on two Euler angles for the case of infinitely thin rods ($I_\parallel=0$) and three Euler angles for the more general case.

We are now ready to define the relevant microscopic field variables and their coarse-grained counterparts. The conven-

tional microscopic definition of the density of mass and center-of-mass momentum are

$$\hat{\rho}(\mathbf{x}) = m\sum_{\alpha} \delta(\mathbf{x}-\mathbf{x}^{\alpha}) \tag{4.7}$$

$$\hat{\mathbf{g}}(\mathbf{x}) = \sum_{\alpha} \mathbf{p}^{\alpha}\delta(\mathbf{x}-\mathbf{x}^{\alpha}), \tag{4.8}$$

which, after coarse graining, result in the macroscopic variables $\rho(\mathbf{x})=[\hat{\rho}(\mathbf{x})]_c$ and $\mathbf{g}(\mathbf{x})=[\hat{\mathbf{g}}(\mathbf{x})]_c \equiv \rho(\mathbf{x})\mathbf{v}(\mathbf{x})$. The last term defines the macroscopic velocity field $\mathbf{v}(\mathbf{x})$. In a similar manner we introduce the macroscopic field $\mathbf{Q}(\mathbf{x})$ of the nematic tensorial order parameter [4,16,19,20], also called the alignment tensor [21]:

$$\frac{\rho(\mathbf{x})}{m}\mathbf{Q}(\mathbf{x}) = \left(\sum_{\alpha} \mathbf{Q}^{\alpha}\delta(\mathbf{x}-\mathbf{x}^{\alpha})\right)_c \tag{4.9}$$

using $\mathbf{Q}^{\alpha}$ from Eq. (4.1). The factor $\rho(\mathbf{x})/m$ is introduced to make $\mathbf{Q}(\mathbf{x})$ unitless. With the microscopic definition for the density of the moment-of-inertia tensor,

$$\begin{aligned}\hat{\mathcal{I}}_{ij}(\mathbf{x}) &= \sum_{\alpha} I_{ij}^{\alpha}\delta(\mathbf{x}-\mathbf{x}^{\alpha}) \\ &= \sum_{\alpha}\left[\Delta I Q_{ij}^{\alpha} + \left(\frac{2}{3}I_{\perp}+\frac{1}{3}I_{\parallel}\right)\delta_{ij}\right]\delta(\mathbf{x}-\mathbf{x}^{\alpha}),\end{aligned} \tag{4.10}$$

we obtain the coarse-grained moment-of-inertia density

$$\mathcal{I}_{ij}(\mathbf{x}) = \frac{\rho(\mathbf{x})}{m}\left[\Delta I Q_{ij}(\mathbf{x}) + \left(\frac{2}{3}I_{\perp}+\frac{1}{3}I_{\parallel}\right)\delta_{ij}\right]. \tag{4.11}$$

Finally, the microscopic field of the density of spin angular momentum is

$$\hat{\mathbf{l}}(\mathbf{x}) = \sum_{\alpha} \mathbf{l}^{\alpha}\delta(\mathbf{x}-\mathbf{x}^{\alpha}). \tag{4.12}$$

Its associated coarse-grained variable is $\mathbf{l}(\mathbf{x})=[\hat{\mathbf{l}}(\mathbf{x})]_c \equiv \boldsymbol{\mathcal{I}}(\mathbf{x})\boldsymbol{\Omega}(\mathbf{x})$, where the last expression defines the macroscopic field $\boldsymbol{\Omega}(\mathbf{x})$ of angular velocity in full analogy to $\mathbf{v}(\mathbf{x})$.

We are interested in the dynamics of the nematic phase where the orientational order is uniaxial. The alignment tensor therefore assumes the form

$$Q_{ij}(\mathbf{x}) = S\left[n_i(\mathbf{x})n_j(\mathbf{x}) - \tfrac{1}{3}\delta_{ij}\right], \tag{4.13}$$

where, on average, the molecules point along the director $\mathbf{n}(\mathbf{x})$. The Maier-Saupe order parameter S is constant in the nematic phase. With the uniaxial $\mathbf{Q}(\mathbf{x})$ of Eq. (4.13), the moment-of-inertia density $\boldsymbol{\mathcal{I}}(\mathbf{x})$ of Eq. (4.11) becomes

$$\mathcal{I}_{ij} = \mathcal{I}_{\parallel}n_i n_j + \mathcal{I}_{\perp}(\delta_{ij} - n_i n_j) \tag{4.14}$$

with

$$\mathcal{I}_{\parallel} = \frac{\rho}{m}\left(\frac{2}{3}I_{\perp}+\frac{1}{3}I_{\parallel}+\frac{2}{3}\Delta I S\right),$$

$$\mathcal{I}_{\perp} = \frac{\rho}{m}\left(\frac{2}{3}I_{\perp}+\frac{1}{3}I_{\parallel}-\frac{1}{3}\Delta I S\right). \tag{4.15}$$

Its anisotropy is quantified by

$$\Delta\mathcal{I} = \mathcal{I}_{\parallel} - \mathcal{I}_{\perp} = \Delta I\frac{\rho}{m}S. \tag{4.16}$$

Note, as indicated in Sec. II, that $\mathcal{I}_{\parallel}=0$ in the limit of infinitely thin rods ($I_{\parallel}=0$) and perfect nematic order ($S=1$).

Thus, our set of dynamic variables is $\{\rho,\mathbf{n},\mathbf{g},\mathbf{l}\}$ for which we must determine all possible Poisson brackets.

B. Poisson brackets

The calculation of the Poisson brackets is straightforward. In addition to the comments about the angular variables in the preceding section and the antisymmetry relation expressed in Eq. (3.3), we use properties of the δ function summarized as

$$\delta(\mathbf{x}-\mathbf{x}') = \delta(\mathbf{x}'-\mathbf{x}), \tag{4.17a}$$

$$f(\mathbf{x})\,\delta(\mathbf{x}-\mathbf{x}') = f(\mathbf{x}')\,\delta(\mathbf{x}-\mathbf{x}'), \tag{4.17b}$$

$$\nabla_i\delta(\mathbf{x}-\mathbf{x}') = -\nabla'_i\delta(\mathbf{x}-\mathbf{x}'), \tag{4.17c}$$

where $\nabla_i=\partial/\partial x_i$, $\nabla'_i=\partial/\partial x'_i$, and $f(\mathbf{x})$ is an arbitrary function including the δ function itself.

In the following, we list all the nonzero Poisson brackets which determine the nondissipative velocities of our dynamic variables. The dynamics of the center-of-mass density $\rho(\mathbf{x})$ is provided by

$$\{\rho(\mathbf{x}), g_i(\mathbf{x}')\} = \nabla_i\delta(\mathbf{x}-\mathbf{x}')\rho(\mathbf{x}'). \tag{4.18}$$

To derive the Poisson brackets of the director, we first calculate the Poisson brackets of the alignment tensor. According to the definition (4.9), we only have a microscopic expression for $\rho(\mathbf{x})\mathbf{Q}(\mathbf{x})$ but not for $\mathbf{Q}(\mathbf{x})$ alone. An analogous, however more complicated, situation occurred in our previous paper [11]. To calculate, e.g., $\{Q_{ij}(\mathbf{x}), g_k(\mathbf{x}')\}$, we apply the product rule for Poisson brackets to $\{\rho(\mathbf{x})Q_{ij}(\mathbf{x}), g_k(\mathbf{x}')\}$ and arrive at

$$\begin{aligned}\{Q_{ij}(\mathbf{x}), g_k(\mathbf{x}')\} &= \frac{1}{\rho(\mathbf{x})}\{\rho(\mathbf{x})Q_{ij}(\mathbf{x}), g_k(\mathbf{x}')\} \\ &\quad - \frac{Q_{ij}(\mathbf{x})}{\rho(\mathbf{x})}\{\rho(\mathbf{x}), g_k(\mathbf{x}')\}.\end{aligned} \tag{4.19}$$

The first term on the right-hand side and the second term, already known from Eq. (4.18), then combine to yield

$$\{Q_{ij}(\mathbf{x}), g_k(\mathbf{x}')\} = \nabla_k\delta(\mathbf{x}-\mathbf{x}')Q_{ij}(\mathbf{x}'). \tag{4.20}$$

In the same manner, we calculate

$$\{Q_{ij}(\mathbf{x}), l_k(\mathbf{x}')\} = -\left[\varepsilon_{ijk}Q_{il}(\mathbf{x}) + \varepsilon_{ikl}Q_{jl}(\mathbf{x})\right]\delta(\mathbf{x}-\mathbf{x}'), \tag{4.21}$$

where we have used the product rule and Eq. (4.5) to evaluate the microscopic Poisson bracket $\{Q_{ij}^{\alpha}, l_k^{\beta}\}$ and the fact that

$\{\rho(\mathbf{x}), l_k(\mathbf{x}')\}=0$. The Poisson brackets for the director now follow by projection from the uniaxial representation (4.13) of the alignment tensor (see Ref. [11] for details):

$$\{n_i(\mathbf{x}), g_j(\mathbf{x}')\} = \frac{1}{S}\delta_{ik}^T\{Q_{kl}(\mathbf{x}), g_j(\mathbf{x}')\}n_l(\mathbf{x}), \tag{4.22}$$

where

$$\delta_{ij}^T = \delta_{ij} - n_i n_j \tag{4.23}$$

is the projector on the space perpendicular to $\mathbf{n}(\mathbf{x})$. The same formula is valid with $g_j(\mathbf{x}')$ replaced by $l_j(\mathbf{x}')$ so that Eqs. (4.20)–(4.23) finally give

$$\{n_i(\mathbf{x}), g_j(\mathbf{x}')\} = [\nabla_j n_i(\mathbf{x})]\delta(\mathbf{x}-\mathbf{x}') \tag{4.24a}$$

$$\{n_i(\mathbf{x}), l_j(\mathbf{x}')\} = -\varepsilon_{ijk}n_k(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}'). \tag{4.24b}$$

Note that the Poisson brackets of $Q_{ij}(\mathbf{x})$ and $n_i(\mathbf{x})$ with $g_k(\mathbf{x}')$ are much simpler in this formulation with spin angular momentum than they are in the alternative one [11,22] in which there is no spin angular momentum and $\mathbf{g}$ is the total rather than the center-of-mass momentum density. In particular, the director-momentum bracket $\lambda_{ijk}\nabla_k\delta(\mathbf{x}-\mathbf{x}')$ that plays such an important role in the latter formulation is not present in the current one.

The reactive velocity of the translational momentum follows from

$$\{g_i(\mathbf{x}), \rho(\mathbf{x}')\} = \rho(\mathbf{x})\nabla_i\delta(\mathbf{x}-\mathbf{x}'), \tag{4.25a}$$

$$\{g_i(\mathbf{x}), n_j(\mathbf{x}')\} = -[\nabla_i n_j(\mathbf{x})]\delta(\mathbf{x}-\mathbf{x}'), \tag{4.25b}$$

$$\{g_i(\mathbf{x}), g_j(\mathbf{x}')\} = -\nabla'_i[\delta(\mathbf{x}-\mathbf{x}')g_j(\mathbf{x}')] + \nabla_j\delta(\mathbf{x}-\mathbf{x}')g_i(\mathbf{x}'), \tag{4.25c}$$

$$\{g_i(\mathbf{x}), l_j(\mathbf{x}')\} = l_j(\mathbf{x})\nabla_i\delta(\mathbf{x}-\mathbf{x}'). \tag{4.25d}$$

Equations (4.25a) and (4.25b) are related to Eqs. (4.18) and (4.24a) by the antisymmetry relation of the Poisson brackets whereas Eqs. (4.25c) and (4.25d) are readily calculated. Again the missing term in the momentum-director bracket compared to Ref. [11] is compensated by the additional Poisson bracket (4.25d).

Finally, the nondissipative dynamics of the angular-momentum density is governed by

$$\{l_i(\mathbf{x}), n_j(\mathbf{x}')\} = -\varepsilon_{ijk}n_k(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}'), \tag{4.26a}$$

$$\{l_i(\mathbf{x}), g_j(\mathbf{x}')\} = l_i(\mathbf{x}')\nabla_j\delta(\mathbf{x}-\mathbf{x}'), \tag{4.26b}$$

$$\{l_i(\mathbf{x}), l_j(\mathbf{x}')\} = -\varepsilon_{ijk}l_k(\mathbf{x}')\delta(\mathbf{x}-\mathbf{x}'). \tag{4.26c}$$

V. NEMATODYNAMICS WITH SPIN ANGULAR MOMENTUM

Following the systematic structure of the theory outlined in Sec. III, we now derive the full set of equations as presented and discussed in Sec. II. We first calculate the reactive and dissipative velocities needed to formulate the dynamic eqations for the set of dynamic variables $\{\rho, \mathbf{n}, \mathbf{g}, \mathbf{l}\}$ and then introduce the spin angular velocity $\mathbf{\Omega}$.

A. Nondissipative velocities

To calculate the nondissipative velocities from Eq. (3.2), we need the Hamiltonian

$$\mathcal{H} = \int\left(\frac{\mathbf{g}^2(\mathbf{x})}{2\rho(\mathbf{x})} + \frac{1}{2}l_i(\mathbf{x})\mathcal{I}_{ij}^{-1}(\mathbf{x})l_j(\mathbf{x})\right)d^3x + F[\rho(\mathbf{x}), \mathbf{n}(\mathbf{x})]. \tag{5.1}$$

It consists of a kinetic part, subdivided into a translational and rotational term, and a free energy $F[\rho(\mathbf{x}), \mathbf{n}(\mathbf{x})] = \int f(\rho, \mathbf{n}, \nabla\mathbf{n})d^3x$, which is Frank's free energy plus a term depending only on ρ. In the following, we will need derivatives of the inverse of the moment-of-inertia density such as $\partial\mathcal{I}_{ij}^{-1}/\partial y$ where y stands for ρ or $\mathbf{n}$. Taking the derivative of $\mathcal{I}_{ij}\mathcal{I}_{jk}^{-1} = \delta_{ik}$ with respect to y, we find

$$\frac{\partial}{\partial y}\mathcal{I}_{ij}^{-1} = -\mathcal{I}_{ik}^{-1}\left(\frac{\partial}{\partial y}\mathcal{I}_{kl}\right)\mathcal{I}_{lj}^{-1}. \tag{5.2}$$

The nondissipative velocity for the density is simply $V^\rho = -\nabla\cdot\mathbf{g}(\mathbf{x})$ which immediately gives the mass-conservation law. For the director, we use the Poisson brackets (4.24) and the fact that $\delta\mathcal{H}/\delta l_j(\mathbf{x}') = \mathcal{I}_{jk}^{-1}l_k = \Omega_j(\mathbf{x}')$ and arrive at

$$V_i^{\mathbf{n}} = -\mathbf{v}(\mathbf{x})\cdot\nabla n_i(\mathbf{x}) + \varepsilon_{ijk}\Omega_j(\mathbf{x})n_k(\mathbf{x}). \tag{5.3}$$

The first term on the right-hand side is the convective derivative of $\mathbf{n}$. The second term introduces a reactive coupling to the angular velocity $\mathbf{\Omega}(\mathbf{x})$. In the purely hydroydnamical model [3,11], this term is replaced by $\lambda_{ijk}\nabla_j v_k$ coupling $\partial n_i/\partial t$ to the symmetric and antisymmetric parts of the deformation-rate tensor $\nabla_i v_j$.

The nondisspative velocity $\mathbf{V}^{\mathbf{g}}$ is calculated with the help of the Poisson brackets (4.25). Applied to the rotational part of the kinetic energy in $\mathcal{H}$, i.e., $\frac{1}{2}l_i(\mathbf{x})\mathcal{I}_{ij}^{-1}(\mathbf{x})l_j(\mathbf{x})$, they produce a contribution $\mathbf{V}_{\mathrm{rot}}^{\mathbf{g}}$ to the non-dissipative velocity $\mathbf{V}^{\mathbf{g}}$ whose terms add up to zero. Specifically, we find

$$V_{\mathrm{rot},i}^{\mathbf{g}} = -\rho\nabla_i\left(\frac{1}{2}l_k l_l\frac{\partial\mathcal{I}_{kl}^{-1}}{\partial\rho}\right) + (\nabla_i n_j)\left(\frac{1}{2}l_k l_l\frac{\partial\mathcal{I}_{kl}^{-1}}{\partial n_j}\right) - l_j\nabla_i\Omega_j, \tag{5.4}$$

which we rewrite as

$$V_{\mathrm{rot},i}^{\mathbf{g}} = \nabla_i\left(\frac{1}{2}\mathcal{I}_{kl}^{-1}l_k l_l\right) - \nabla_i\left(\rho\frac{1}{2}l_k l_l\frac{\partial\mathcal{I}_{kl}^{-1}}{\partial\rho}\right) - \nabla_i(l_j\Omega_j). \tag{5.5}$$

Using Eq. (5.2) to evaluate the derivative with respect to ρ and the fact that $\mathcal{I}_{kl}$ is linear in ρ [see Eqs. (4.14) and (4.15)], one shows immediately that the three terms add up to zero, i.e., $\mathbf{V}_{\mathrm{rot}}^{\mathbf{g}}=0$. All the other contributions to $\mathbf{V}^{\mathbf{g}}$ can be written in a compact form,

$$V_i^{\mathbf{g}} = -\nabla_j\left(\frac{g_i(\mathbf{x})g_j(\mathbf{x})}{\rho(\mathbf{x})}\right) - \nabla_i p + \nabla_j \sigma_{ij}^E, \tag{5.6}$$

as explained in Ref. [11]. The first term on the right-hand side introduces the momentum flux tensor, the second term contains the pressure p, and $\boldsymbol{\sigma}^E$ is the Ericksen stress tensor,

$$\sigma_{ij}^E = -\frac{\partial f}{\partial \nabla_j n_k}\nabla_i n_k. \tag{5.7}$$

Note that compared to Ref. [11] a term that contains the molecular field $\delta F/\delta \mathbf{n}$ is completely missing.

Finally the Poisson brackets (4.26) give the reactive velocity of the angular-momentum density,

$$V_i^{\mathbf{l}} = \varepsilon_{ijk} n_k(\mathbf{x})\left(\frac{1}{2} l_r l_s \frac{\partial \mathcal{I}_{rs}^{-1}}{\partial n_j} + \frac{\delta F}{\delta n_j(\mathbf{x})}\right) - \nabla_j[l_i(\mathbf{x}) v_j(\mathbf{x})] + \varepsilon_{ijk}\Omega_j(\mathbf{x}) l_k(\mathbf{x}). \tag{5.8}$$

Again, one can show using Eqs. (4.14) and (5.2) that the first and the fourth term on the right-hand side resulting from the rotational kinetic energy cancel each other so that we obtain

$$V_i^{\mathbf{l}} = -\nabla_j[l_i(\mathbf{x}) v_j(\mathbf{x})] + \varepsilon_{ijk} n_k(\mathbf{x})\frac{\delta F}{\delta n_j(\mathbf{x})}. \tag{5.9}$$

The first term introduces the angular momentum flux tensor in full analogy to the linear momentum and the second term is a coupling to the molecular field.

B. Dissipative velocities and final equations

1. Center-of-mass density

For the conserved center-of-mass density, dissipative velocities are not allowed, and the mass-conservation law follows:

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla}\cdot\mathbf{g}. \tag{5.10}$$

2. Director

The time derivative $\partial \mathbf{n}/\partial t$ couples dissipatively only to forces conjugate to fields, $\mathbf{n}$ and ρ with the same sign under time reversal as $\mathbf{n}$. A dissipative term proportional to $\mathbf{n}\delta\mathcal{H}/\delta\rho$, which has the correct sign under time reversal, cannot occur because it is always perpendicular to $\partial \mathbf{n}/\partial t$ [11]. A second dissipative term introduces a coupling to $\delta\mathcal{H}/\delta n_i$ with a dissipative tensor δ_{ij}^T/γ, where the projector δ_{ij}^T defined in Eq. (4.23) ensures that $\partial \mathbf{n}/\partial t$ is perpendicular to $\mathbf{n}$ and γ is a rotational viscosity. Together with Eq. (5.3), the dynamic equation for the director then reads

$$\frac{\partial n_i}{\partial t} = -\mathbf{v}\cdot\boldsymbol{\nabla} n_i + \varepsilon_{ijk}\Omega_j n_k - \frac{1}{\gamma}\delta_{ij}^T\left(\frac{1}{2} l_k l_l \frac{\partial \mathcal{I}_{kl}^{-1}}{\partial n_j} + \frac{\delta F}{\delta n_j}\right). \tag{5.11}$$

With the definition of the components of the molecular field, $h_i = -\delta_{ij}^T \delta F/\delta n_j$, and the expression

$$\delta_{ij}^T \frac{1}{2} l_k l_l \frac{\partial \mathcal{I}_{kl}^{-1}}{\partial n_j} = -(\mathcal{I}_\parallel - \mathcal{I}_\perp)\Omega_\parallel \boldsymbol{\Omega}_\perp, \tag{5.12}$$

which we derive with the help of Eqs. (4.14) and (5.2) and $l_i = \mathcal{I}_{ij}\Omega_j$, we finally arrive at the director equation as presented in Eq. (2.3) in Sec. II.

3. Spin angular momentum density

The fields $\delta\mathcal{H}/\delta l_i = \Omega_i$ and $\delta\mathcal{H}/\delta g_i = v_i$ have the same sign under time reversal as $\mathbf{l}$ and can contribute terms of the equation for $\partial \mathbf{l}/\partial t$. To determine the form of these terms, it is important to realize that $\mathbf{l}$ and $\boldsymbol{\Omega}$ are pseudovectors that do not change sign under space inversion but that the momentum density, $\mathbf{g}$, and the velocity, $\mathbf{v}$, are vectors that do change sign under space inversion. Thus a term directly proportional to v_i in the equation for $\partial l_i/\partial t$ is prohibited but one proportional to Ω_i is not. Pseudovectors that are even under $\mathbf{n}\to-\mathbf{n}$ can be constructed from the spatial derivatives of $\mathbf{v}$ and the director. Thus we look for dissipative terms containing these pseudovector combinations of $\nabla_i v_j$. The first pseudovector is $\omega_i = \varepsilon_{ijk}\nabla_j v_k/2$. Together with the angular velocity, it gives rise to the dissipative term $-\Gamma_{ij}^{\Omega}(\Omega_j - \omega_j)$ whose form is dictated by the requirement that during a uniform rotation of the whole sample ($\boldsymbol{\Omega} = \boldsymbol{\omega}$) no energy is dissipated. A second pseudovector of the velocity, which preserves the $\mathbf{n}\to-\mathbf{n}$ symmetry of the nematic phase, is $\frac{1}{2}(\varepsilon_{ijl} n_l n_k + \varepsilon_{ikl} n_l n_j)A_{jk}$, where $A_{jk} = (\nabla_j v_k + \nabla_k v_j)/2$ stands for the symmetrized velocity gradient. Furthermore, the third-rank tensor in front of A_{jk} is symmetric in j and k, which is important for the next paragraph where we use the Onsager principle to find the dissipative velocities for the momentum density. Introducing the dissipative torque

$$\tau_i' = -\Gamma_{ij}^{\Omega}(\Omega_j - \omega_j) - \frac{\Gamma^A}{2}(\varepsilon_{ijl} n_l n_k + \varepsilon_{ikl} n_l n_j)A_{jk}, \tag{5.13}$$

where

$$\Gamma_{ij}^{\Omega} = \Gamma_\parallel^{\Omega} n_i n_j + \Gamma_\perp^{\Omega}(\delta_{ij} - n_i n_j) \tag{5.14}$$

obeys the uniaxial symmetry of the nematic phase, and combining it with Eq. (5.9), we arrive at the formula describing the dynamics of $\mathbf{l}$,

$$\frac{\partial l_i}{\partial t} = -\nabla_j(l_i v_j) + \varepsilon_{ijk} n_k \frac{\delta F}{\delta n_j} + \tau_i'. \tag{5.15}$$

To replace $\mathbf{l}$ by the angular velocity, we write

$$\mathbf{l} = \mathcal{I}_\parallel \Omega_\parallel \mathbf{n} + \mathcal{I}_\perp \boldsymbol{\Omega}_\perp. \tag{5.16}$$

The time derivative of $\mathbf{l}$ involves $\partial\mathcal{I}_\alpha/\partial t$, where α represents $\parallel$ or $\perp$. We find

$$\frac{\partial \mathcal{I}_\alpha}{\partial t} = \frac{\partial \mathcal{I}_\alpha}{\partial \rho}\frac{\partial \rho}{\partial t} = -\nabla_i(\mathcal{I}_\alpha v_i), \tag{5.17}$$

where we used the fact that $\mathcal{I}_\alpha$ linearly depends on ρ [see Eq. (4.15)] and where we also employed the mass-conservation law $\partial\rho/\partial t = -\nabla_i(\rho v_i)$. With Eq. (5.17) and the definition of the total time derivative, $d/dt = \partial/\partial t + v_i\nabla_i$, it is straightforward to show that

$$\frac{\partial l_i}{\partial t} + \nabla_j (l_i v_j) = \mathcal{I}_\perp \frac{d\mathbf{\Omega}_\perp}{dt} + \Omega_\parallel \frac{d\mathbf{n}}{dt} + \mathbf{n}\frac{d\Omega_\parallel}{dt}. \quad (5.18)$$

We introduce this term into the balance equation (5.15) for $\mathbf{l}$ and project it on $\mathbf{n}$ and the plane perpendicular to $\mathbf{n}$ to finally arrive at the respective Eqs. (2.5) and (2.4) in Sec. II. In deriving the last two terms of Eq. (2.5), we also used $\mathbf{n}\cdot d\Omega_\perp/dt = -(d\mathbf{n}/dt)\cdot\Omega_\perp$ and replaced $d\mathbf{n}/dt$ by Eq. (2.3)

4. Center-of-mass momentum density

The dissipative term of the momentum balance is determined by the viscous stress tensor $\boldsymbol{\sigma}'$, which couples again to Ω_i and $\nabla_i v_j$ as in the preceding paragraph. The form of the dissipative part of the stress tensor is subject to restrictions. First of all, because the total angular momentum (spin plus center-of-mass) is conserved, the antisymmetric part $\boldsymbol{\sigma}^{A\prime}$ of the viscous stress tensor and the dissipative torque $\boldsymbol{\tau}'$ of Eq. (5.13) are related (see Appendix B):

$$\sigma_{ij}^{A\prime} = -\tfrac{1}{2}\varepsilon_{ijk}\tau_k' = \tfrac{1}{2}\varepsilon_{ijk}\Gamma_{kl}^{\Omega}(\Omega_l - \omega_l) + \tfrac{1}{2}\Gamma^A(n_j A_{in} n_n - n_i A_{jn} n_n). \quad (5.19)$$

To construct the symmetric part $\boldsymbol{\sigma}^{S\prime}$ of the viscous stress tensor, we use Onsager's principle. It says that the dissipative fluxes $\boldsymbol{\tau}'$, $\boldsymbol{\sigma}^{S\prime}$ are coupled to the generalized forces $\mathbf{\Omega}-\boldsymbol{\omega}$, $\mathbf{A}$ by a symmetric, dissipative tensor. In symbolic notation this means

$$\begin{pmatrix} -\boldsymbol{\tau}' \\ \boldsymbol{\sigma}^{S\prime} \end{pmatrix} = \begin{pmatrix} \mathbf{\Gamma}^{\Omega} & \Gamma^A \boldsymbol{\varepsilon}\mathbf{nn} \\ \Gamma^A(\boldsymbol{\varepsilon}\mathbf{nn})^t & \boldsymbol{\alpha} \end{pmatrix} \begin{pmatrix} \mathbf{\Omega}-\boldsymbol{\omega} \\ \mathbf{A} \end{pmatrix}, \quad (5.20)$$

where the superscript t in $(\boldsymbol{\varepsilon}\mathbf{nn})^t$ stands for the appropriately transposed third-rank tensor $\boldsymbol{\varepsilon}\mathbf{nn}$ of Eq. (5.13). The first line of the tensor equation reproduces the dissipative torque (5.13), the second line gives

$$\sigma_{ij}^{S\prime} = \alpha_{ijkl}A_{kl} + \tfrac{1}{2}\Gamma^A(\varepsilon_{ilk}n_j n_l + \varepsilon_{jlk}n_i n_l)(\Omega_k - \omega_k), \quad (5.21)$$

where the viscosity tensor $\boldsymbol{\alpha}$ has the usual form required by the uniaxial symmetry of our medium (see, e.g., Ref. [11]),

$$\begin{aligned}\alpha_{ijkl} = {} & \alpha_1 n_i n_j n_k n_l + \frac{\alpha_4}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ & + \frac{\alpha_5+\alpha_6}{4}(n_i n_k \delta_{jl} + n_j n_k \delta_{il} + n_i n_l \delta_{jk} + n_j n_l \delta_{ik}) \\ & + \zeta_1 \delta_{ij}\delta_{kl} + \zeta_2(\delta_{ij} n_k n_l + n_i n_j \delta_{kl}). \end{aligned} \quad (5.22)$$

Adding up reactive and dissipative terms, the momentum balance finally reads

$$\frac{\partial g_i}{\partial t} = -\nabla_j\left(\frac{g_i g_j}{\rho}\right) - \nabla_i p + \nabla_j(\sigma_{ij}^E + \sigma_{ij}^{S\prime} + \sigma_{ij}^{A\prime}). \quad (5.23)$$

The complete set of equations of nematodynamics including the spin angular momentum is reproduced in Eqs. (2.1)–(2.9). The Leslie-Ericksen and hydroydnamic limits of these equations are derived in Sec. II.

ACKNOWLEDGMENTS

One of the authors (H.S.) acknowledges financial support from the Deutsche Forschungsgemeinschaft under Grant No. Sta 352/5-1 and through the International Graduate College "Soft Matter." One of the authors (T.C.L.) was supported by the U.S. National Science Foundation under Grant No. DMR04-05187.

APPENDIX A: NONLINEARITIES IN RIGID-BODY MOTION

Our equation for the director reduces to that for the anisotropy axis $\mathbf{n}$ for a single uniaxial rigid body if $\mathbf{n}(\mathbf{x})$ is independent of $\mathbf{x}$ and $\mathbf{h}=\mathbf{0}$. If $\Gamma_{ij}^{\Omega}=0$ and $\Gamma^A=0$, spin angular momentum is conserved [see Eq. (5.15)], i.e., $d\mathbf{L}/dt = d/dt(\int d^3x \mathbf{l}) = \mathbf{0}$, and $\Omega_\parallel = L_\parallel/\tilde{I}_\parallel$ and $\mathbf{\Omega}_\perp = \mathbf{L}_\perp/\tilde{I}_\perp$ where $\tilde{I}_{\parallel,\perp} = \int d^3x \mathcal{I}_{\parallel,\perp}$. The equation of motion for the anisotropy axis is then

$$\frac{d\mathbf{n}}{dt} = \mathbf{\Omega}\times\mathbf{n} + \frac{\Delta\mathcal{I}}{\gamma}\Omega_\parallel \mathbf{\Omega}_\perp. \quad (A1)$$

This equation has a dissipative term implying that energy is not conserved even though spin angular momentum is. Since $\mathbf{L}$ is a constant, we can choose it to be a vector $L\mathbf{e}_z$ of fixed length pointing along the space fixed unit vector $\mathbf{e}_z$ along the z axis. When $\mathbf{n}=(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is expressed in polar coordinates relative to the z axis, Eq. (A1) reduces to the equations

$$\frac{d\phi}{dt} = \frac{L}{\tilde{I}_\perp}, \quad (A2)$$

$$\frac{d\theta}{dt} = -\frac{1}{2\gamma}\frac{\Delta\mathcal{I}}{\tilde{I}_\parallel \tilde{I}_\perp} L^2 \sin 2\theta. \quad (A3)$$

The equation for θ is easily solved subject to the boundary condition that $\theta(t=0)=\theta_0$,

$$\tan\theta(t) = \tan\theta_0 \exp\left(-\frac{1}{4\gamma}\frac{\Delta\mathcal{I}}{\tilde{I}_\parallel\tilde{I}_\perp}L^2 t\right). \quad (A4)$$

Thus, if $\mathcal{I}_\parallel > \mathcal{I}_\perp$, $\theta(t)\to 0$ if $0 \leq \theta_0 < \pi/2$ or $\theta(t)\to\pi$ if $\pi/2 < \theta_0 \leq \pi$ as $t\to\infty$. This means that $\mathbf{n}$ will align or antialign with the angular momentum direction and that the angular momentum comes entirely from spinning parallel to the anisotropy axis with kinetic energy $L^2/(2\tilde{I}_\parallel)$. If $\mathcal{I}_\parallel < \mathcal{I}\perp$, $\theta(t)\to\pi/2$ for $0<\theta_0<\pi$. In this case, $\mathbf{n}$ lies in the xy plane and rotates according to Eq. (A2), and the kinetic energy is $L^2/(2\tilde{I}_\perp)$. Thus, when angular momentum is conserved but energy is not, the rigid body will evolve toward the state with the lowest kinetic energy consistent with the constraint of fixed angular momentum.

APPENDIX B: TORQUES AND STRESS TENSOR

Here we shortly demonstrate that the antisymmetric part of the stress tensor is equivalent to a torque acting on the

intrinsic angular momentum. The total angular momentum of a system with volume V is given by

$$\mathbf{L} = \int_V (\rho \mathbf{x} \times \mathbf{v} + \mathbf{l}) d^3x. \tag{B1}$$

In case of zero body forces and torques (which might originate from applied magnetic and electric fields or gravitation), only surface forces can change the total angular momentum. Per definition they are described by the stress tensor σ so that

$$\frac{d\mathbf{L}}{dt} = \int_V \mathbf{x} \times \boldsymbol{\sigma} d\mathbf{f}, \tag{B2}$$

where ∂V means surface of V. Applying Gauss's theorem to the right-hand side results in

$$\frac{d\mathbf{L}}{dt} = \int_{\partial V} (\mathbf{x} \times \text{div } \boldsymbol{\sigma} + \boldsymbol{\tau}) d^3x, \tag{B3}$$

where we introduced the torque

$$\tau_i = -\varepsilon_{ijk}\sigma_{jk}. \tag{B4}$$

With

$$\frac{d\mathbf{L}}{dt} = \int_V \left(\rho \mathbf{x} \times \frac{d\mathbf{v}}{dt} + \frac{d\mathbf{l}}{dt} \right) \tag{B5}$$

and the momentum balance in differential form,

$$\rho \frac{d\mathbf{v}}{dt} = \text{div } \boldsymbol{\sigma}, \tag{B6}$$

we obtain from Eq. (B3)

$$\frac{d\mathbf{l}}{dt} = \boldsymbol{\tau}, \tag{B7}$$

where τ is the torque acting on $\mathbf{l}$.

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