Dynamics of dissipative ordered fluids

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A variational principle is proposed that allows to derive the equations of motion for a fluid with a general microstructure described by a tensorial order parameter. The only constitutive ingredients are the densities of the free energy and the dissipation, both subject to appropriate invariance requirements. As an illustration, it is shown how the hydrodynamic theory for uniaxial nematic liquid crystals can be derived within this setting.

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I. INTRODUCTION

Many *soft* materials can be modeled as fluids with a tensorial order parameter. The clearest example of these is perhaps a nematic liquid crystal, whose biaxial states, which preferably occur around defects or under shear, are described by a second-rank alignment tensor (see, e.g., [1], Chap. 2 and [2]). When the nematic is uniaxial with constant scalar order parameter, it can be described by a *director*, and its dynamics has long been understood in terms of balances of linear and angular momenta, also including the microstructure of the local material element [3–5]. Moreover, the dynamics of uniaxial nematics with variable scalar order was treated in depth by Ericksen [6]. However, a rational systematic theory to arrive at the evolution equations for more general dissipative microstructures is still missing. Presumably, this is so because simply balancing linear and angular momenta does not suffice to predict the evolution of the system when the microstructure fails to be vectorial.

Various avenues have already been taken to arrive at particular equations for the full second-rank alignment tensor. Using methods of nonequilibrium thermodynamics, Hess [2,7] proposed a theory, which was later generalized by Hess and Pardowitz to include spatial variations [8] (see also [9,10] for the homogeneous case and [11,12] for a discussion of the foundations of this approach). A further extension of this model was considered in [13,14]. In a different vein, starting from a Fokker-Planck equation for the orientational distribution function proposed by Hess [15], several authors used closure approximations to obtain evolution equations for the second-rank alignment tensor [15–17]. More recently, plastic flow has been studied [18] by using a fourth-rank tensor to describe the order, which calls once more for a general theory of ordered fluids.

For uniaxial nematics, one way to arrive at the equations of motion without positing balance equations was pointed out by Vertogen [19]. His development is based on an analogy with classical Lagrange mechanics with Rayleigh dissipation. While this analogy is sufficient to derive the viscous stress, it gives neither the elastic stress nor the couple stress, and no information is gained regarding proper boundary conditions at free surfaces. Furthermore, the equations of motion for the flow and the director are treated in somewhat different ways, see also [20], p. 145.

Here we propose a general theory for dissipative fluids described by an order tensor of arbitrary rank. Rather than positing by analogy the evolution equations, we arrive at them from a variational principle, which, when applied to mass-point dynamics, gives the classical Lagrange-Rayleigh equations. For continua, this theory leads to the evolution equations along with the appropriate boundary conditions.

This principle is posited in Sec. II. In Sec. III, we apply it to a class of continua with dissipative microstructure: this class is chosen so as to encompass nematic liquid crystals, among many other materials. We arrive at a set of general dynamical equations, and we show how these can subsume the balance equations for linear and angular momenta. One advantage of our method is that it introduces only few constitutive laws: both elastic and viscous stresses, for example, are obtained from the elastic and dissipated energies.

For simplicity, here we generally consider unconstrained order tensors; special constraints can be treated with the aid of appropriate Lagrange multipliers. They are needed in the case illustrated in Sec. IV, where we show, as an example, how the well-known balance equations of nematodynamics can be retraced within the theory presented here. A generalization of our method to fluids with arbitrary order parameters on differentiable manifolds is described in [21].

II. VARIATIONAL PRINCIPLE

We aim at extending to a class of dissipative ordered media the method originally put forward by Rayleigh to describe dissipative discrete systems [22]. The essence of Rayleigh's approach is to balance all generalized forces in Lagrange equations, including inertia, against frictional forces that derive from a dissipation function and are linear in the generalized velocities. We first illustrate this basic balance taking a holonomic dynamical system as a paradigm and then further confining attention to systems subject to conservative active forces. In general, a variational principle allows one to arrive directly at the equations of motion including the appropriate dissipative terms. This principle will be applied in Sec. III to a variety of dissipative ordered fluids.

A. Basic balance

Essentially, our development rests on two assumptions: first, that the total mechanical power, excluding dissipation, can be written as the product of generalized forces by gen-

eralized velocities, and second that these forces are balanced by frictional forces that possess a quadratic velocity potential.

Consider a holonomic dynamical system described by m generalized coordinates $q_1, \ldots, q_m$. We denote by q and $\dot{q}$ the vectors in $\mathbb{R}^m$ of the generalized coordinates and the generalized velocities. We assume that the total mechanical power $\mathcal{W}$ can be written as

$$\mathcal{W} = X \cdot \dot{q} = \sum_{i=1}^{m} X_i \dot{q}_i, \tag{1}$$

where X_i are the generalized forces, including inertia. To help in identifying the generalized forces, we may suppose that X remains unchanged under time reversal, while $\dot{q}$ changes its sign.

When in addition to the mechanical forces X, the system is subject to dissipation, frictional generalized forces Y are also at work that satisfy the balance equation

$$X + Y = 0. \tag{2}$$

Here we make the constitutive assumption that the forces Y are linear in the velocities $\dot{q}$ and that they can be derived from a positive-definite quadratic form $\mathcal{R}$ according to

$$Y = \frac{\partial \mathcal{R}}{\partial \dot{q}}. \tag{3}$$

The velocity potential $\mathcal{R}$ is called the Rayleigh *dissipation function*. The equations of motion are then obtained by inserting Eq. (3) into Eq. (2) as

$$X + \frac{\partial \mathcal{R}}{\partial \dot{q}} = 0. \tag{4}$$

Taking the inner product of both sides of Eq. (4) with $\dot{q}$ yields the balance of energy in the form

$$\mathcal{W} + 2\mathcal{R} = 0, \tag{5}$$

since $\mathcal{R}$ is a homogeneous function of degree two, for which

$$\frac{\partial \mathcal{R}}{\partial \dot{q}} \cdot \dot{q} = 2\mathcal{R}. \tag{6}$$

Sometimes the *total dissipation* $\mathcal{D}$ is used in Eq. (5) instead of $2\mathcal{R}$.

B. Conservative forces

When all active forces are conservative the total mechanical power $\mathcal{W}$ can be written as the rate of change of the total mechanical energy $\mathcal{F}$. Let $V = V(q)$ be the potential energy of the system and $T = T(q, \dot{q})$ its kinetic energy, which is assumed to be a positive-definite quadratic form in the velocities $\dot{q}$. A standard computation yields

$$\dot{\mathcal{F}} = \dot{T} + \dot{V} = \sum_{i=1}^{m} \left(\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} \right) \dot{q}_i, \tag{7}$$

with the Lagrange function $L = T - V$, and so the generalized forces conjugate to the velocities $\dot{q}$ are here found to be

$$X = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q}. \tag{8}$$

The equations of motion (4) then read simply as

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} + \frac{\partial R}{\partial \dot{q}} = 0, \tag{9}$$

which is the standard text-book form (cf., e.g., [23], p. 231). Clearly, the energy balance (5) still holds with $\mathcal{W} = \dot{\mathcal{F}}$.

It should be noticed that, since T is a positive-definite quadratic form in $\dot{q}$ and V is independent of $\dot{q}$, by Eq. (8) X is linear in $\ddot{q}$ and

$$\det \frac{\partial X}{\partial \ddot{q}} \neq 0;$$

thus $\ddot{q}$ can also be expressed in terms of X, q, and $\dot{q}$ as

$$\ddot{q} = B(q, \dot{q}) X + a(q, \dot{q}) \tag{10}$$

(cf. [23], p. 40), where B is an invertible matrix in $\mathbb{R}^{m \times m}$ and d is a vector in $\mathbb{R}^m$.

C. Variational formulation

To generalize Eq. (4) so as to encompass continua, one can argue that the partial derivative of the dissipation function has to be replaced by a functional derivative. However, care has to be taken in appropriately identifying the generalized forces in the bulk and on the boundary.

We show here how the discrete case (4) can be derived from an appropriate variational principle for $\mathcal{R}$, where the configuration remains unchanged, while both the velocities $\dot{q}$ and the accelerations $\ddot{q}$ are subject to judiciously constrained variations. This principle can then directly be applied to continua and it indeed yields the recipe outlined in the preceding paragraph.

For a given configuration we conceive a system of variations $\delta\dot{q}$ of the actual velocity vector $\dot{q}$ that leaves both the generalized forces X and their power $\mathcal{W}$ unchanged. This implies variations $\delta\ddot{q}$ of $\ddot{q}$ to be chosen accordingly: they eventually result in linear combinations of the variations $\delta\dot{q}$, cf. Eq. (10). The constraint on the power input $\mathcal{W}$ can then be treated in the standard way through a Lagrange multiplier, so that $\dot{q}$ may be arbitrarily perturbed.

In the actual evolution of the system through a given configuration, $\dot{q}$ is such that $\mathcal{R}$ attains its minimum relative to all virtual values it can achieve, once both the forces X and their power $\mathcal{W}$ are *frozen* in their actual state. This is a principle of

minimum restrained dissipation, which in a similar form has also been used in irreversible thermodynamics [24,25]. We first require $\mathcal{R}$ to be stationary with respect to this special class of variations. This leads to

$$\delta\mathcal{R}+\lambda\,\delta\mathcal{W}=\left(\frac{\partial\mathcal{R}}{\partial\dot{q}}+\lambda X\right)\cdot\delta\dot{q}=0 \tag{11}$$

for all variations $\delta\dot{q}$, where λ is a Lagrange multiplier. Since $\delta\dot{q}$ is arbitrary, Eq. (11) amounts to

$$\lambda X+\frac{\partial\mathcal{R}}{\partial\dot{q}}=0. \tag{12}$$

The value of λ can be determined by taking the inner product of both sides of Eq. (12) with $\dot{q}$ and requiring the energy balance (5) to hold. This shows that $\lambda=1$, and the stationarity conditions for $\mathcal{R}$ in Eq. (12) just become the equations of motion (4). These are indeed minimality conditions for $\mathcal{R}$ constrained to the linear subspace where both X and $\mathcal{W}$ are prescribed, for $\mathcal{R}$, being a positive-definite quadratic form of $\dot{q}$, has there a minimizer as the unique stationary point.

III. DISSIPATIVE MICROSTRUCTURES

In this section we apply to ordered fluids the variational principle stated in the preceding section. Our aim is to arrive at the evolution equations for a class of dissipative microstructures by positing in each case the appropriate energy and dissipation functionals, which in our development are the only relevant constitutive quantities for these materials.

We consider a continuum that occupies the region $\mathcal{B}$ in space with smooth boundary $\partial\mathcal{B}$, bearing an additional microstructure described by an order tensor $\mathbb{O}$. Here the order parameter space is the linear space of all nth-rank tensors. Though the theory we present can equally be developed by letting the order tensor vary on a differentiable manifold, the gain in generality is little compared with the growth in the mathematical apparatus [21]. On the other hand, as shown in Sec. IV, constraints on $\mathbb{O}$ can generally be treated by means of appropriate Lagrange multipliers (see also [26] and [27]). In our setting, the natural candidates for the generalized velocities are the mass velocity $\boldsymbol{v}$ and the material time derivative

$$\dot{\mathbb{O}}=\frac{\partial}{\partial t}\mathbb{O}+(\boldsymbol{\nabla}\mathbb{O})\boldsymbol{v} \tag{13}$$

of the order tensor $\mathbb{O}$. In Cartesian components,

$$\dot{O}_I=\frac{\partial}{\partial t}O_I+O_{I,j}v_j,$$

where a comma denotes differentiation with respect to a space variable, the summation convention for repeated indices applies, and I is a multi-index, $I=(I_1,\ldots,I_n)$.

The dissipation function characterizes frictional processes that are intrinsic to the material and that should therefore be independent of the observer. This requires the dissipation function to be invariant under all changes of frame, represented by Euclidean transformations acting on all position vectors $\boldsymbol{x}$ as

$$\boldsymbol{x}^*=\mathbf{Q}(t)\boldsymbol{x}+\boldsymbol{b}(t), \tag{14}$$

where $\mathbf{Q}$ is an orthogonal tensor and $\boldsymbol{b}$ a vector, both arbitrarily depending on time. The dissipation function will be automatically invariant, when it is built using only *indifferent* tensors, i.e., those tensors that transform in the usual way under the change of frame (14), see, e.g., [28], Chap. 1. One example is the *shearing* tensor

$$\mathbf{D}=\tfrac{1}{2}[\boldsymbol{\nabla}\boldsymbol{v}+(\boldsymbol{\nabla}\boldsymbol{v})^T],$$

as one finds that $\mathbf{D}^*=\mathbf{Q}(t)\mathbf{D}\mathbf{Q}(t)^T$. Apart from $\mathbf{D}$, we further need an indifferent time derivative of the order tensor $\mathbb{O}$. The simplest one is the *corotational* derivative $\mathring{\mathbb{O}}$. It describes how the order changes in a frame that is rotating with the body. In Cartesian components, it can be written as

$$\mathring{O}_I=\dot{O}_I-\sum_{k=1}^{n}W_{I_kj}O_{I_k^j}, \tag{15}$$

where

$$\mathbf{W}=\tfrac{1}{2}[\boldsymbol{\nabla}\boldsymbol{v}-(\boldsymbol{\nabla}\boldsymbol{v})^T]$$

is the *vorticity* tensor and, for any given multi-index I, $I_k^j=(I_1,\ldots,,I_{k-1},j,I_{k+1},\ldots,I_n)$ is the same multi-index as I, apart from having j as kth-entry. In Eq. (15) the sum clearly extends over all entries of I.

A more general frame-indifferent rate of $\mathbb{O}$ is the *codeformational* time derivative

$$\hat{O}_I=\mathring{O}_I+\sum_{k=1}^{n}a_kD_{I_kj}O_{I_k^j}. \tag{16}$$

Here the coefficients a_k are somehow constitutive: they determine to what extent the deformation of the fluid affects the microstructure. In general, when $\mathbb{O}$ enjoys symmetry properties, these are also inherited by its rate, and special relations among the a_k could be required. Furthermore, when restrictions on some traces of $\mathbb{O}$ exist, additional terms will enter Eq. (16) to make these restrictions preserved in time.

A. Power input

We write the total energy stored in $\mathcal{B}$ as

$$\mathcal{F}=\int_{\mathcal{B}}F\,dV$$

with

$$F=\rho[\tfrac{1}{2}\boldsymbol{v}^2+\phi+\sigma(\rho)+\kappa(\mathbb{O},\dot{\mathbb{O}})+\chi(\mathbb{O})]+W(\mathbb{O},\boldsymbol{\nabla}\mathbb{O}), \tag{17}$$

where ρ is the mass density, ϕ is the potential energy per unit mass of a body force $\boldsymbol{f}=-\boldsymbol{\nabla}\phi$, σ is the potential energy associated with the compressibility of the material, κ is the kinetic energy of the microstructure, taken to be a quadratic form of $\dot{\mathrm{O}}$, χ is the potential energy for the external actions exerted on O, and W is the elastic energy connected with the microstructure. W will in general be required to be frame-indifferent (see Sec. III C below). While the elastic energy might in principle depend also on higher gradients of the order tensor O, to keep the following discussion simple, we take into account only first gradients. The inclusion of higher gradients is feasible within our setting, but it would also require the introduction of higher order forces and moments in the bulk and on the surface [29]. The main features of our method are already evident with an energy density of the form (17).

We write the balance of mass in the usual way, that is,

$$\dot{\rho}+\rho\,\mathrm{div}\,\boldsymbol{v}=0. \tag{18}$$

Then, by the transport theorem, the time rate of $\mathcal{F}$ is

$$\dot{\mathcal{F}}=\int_{\mathcal{B}}\left\{\rho(\dot{\boldsymbol{v}}-\boldsymbol{f})\cdot\boldsymbol{v}+\rho\mathbb{M}\cdot\dot{\mathrm{O}}+\left(\rho\frac{\partial\chi}{\partial\mathrm{O}}+\frac{\partial W}{\partial\mathrm{O}}\right)\cdot\dot{\mathrm{O}}+\frac{\partial W}{\partial\boldsymbol{\nabla}\mathrm{O}}\cdot(\boldsymbol{\nabla}\mathrm{O})^{\cdot}+(W-\rho^2\sigma')\mathrm{div}\,\boldsymbol{v}\right\}dV, \tag{19}$$

where $\sigma':=d\sigma/d\rho$, and use has been made of the fact that κ is a quadratic function of $\dot{\mathrm{O}}$ in arranging the microinertia per unit mass in the form

$$\mathbb{M}:=\left(\frac{\partial\kappa}{\partial\dot{\mathrm{O}}}\right)^{\cdot}-\frac{\partial\kappa}{\partial\mathrm{O}} \tag{20}$$

(cf. (7) and see also [27], p. 19). At variance with the Lagrangian paradigm, here $\dot{\mathcal{F}}$ fails to be the total power input for the system; it must be supplemented with the *surface* power $\mathcal{W}^s$, which for a movable boundary $\partial\mathcal{B}$ takes the general form

$$\mathcal{W}^s=\int_{\partial\mathcal{B}}\{\boldsymbol{X}^s\cdot\boldsymbol{v}+\mathbb{X}^s\cdot\dot{\mathrm{O}}\}dA, \tag{21}$$

where $\boldsymbol{X}^s$, $\mathbb{X}^s$ are generalized external forces associated with the velocities $\boldsymbol{v}$ and $\dot{\mathrm{O}}$, respectively. While $\boldsymbol{X}^s$ is a vector in the ordinary space, $\mathbb{X}^s$ is an nth-rank tensor. Often the surface power derives from a surface potential, i.e., it can be represented as

$$\mathcal{W}^s=\frac{d}{dt}\int_{\partial\mathcal{B}}W^s(\boldsymbol{x},\mathrm{O})dA,$$

where W^s is a scalar function of the position in space $\boldsymbol{x}$ and the order tensor O; clearly, in such a case

$$\boldsymbol{X}^s=\frac{\partial W^s}{\partial\boldsymbol{x}}\quad\text{and}\quad\mathbb{X}^s=\frac{\partial W^s}{\partial\mathrm{O}}.$$

After some integrations by parts in Eq. (19), by use of

$$(\boldsymbol{\nabla}\mathrm{O})^{\cdot}=\boldsymbol{\nabla}\dot{\mathrm{O}}-(\boldsymbol{\nabla}\mathrm{O})\boldsymbol{\nabla}\boldsymbol{v}, \tag{22}$$

the total power input can be cast in the form

$$\dot{\mathcal{F}}+\mathcal{W}^s=\int_{\mathcal{B}}\{\boldsymbol{X}\cdot\boldsymbol{v}+\mathbb{X}\cdot\dot{\mathrm{O}}\}dV+\int_{\partial\mathcal{B}}\{(\boldsymbol{X}^b+\boldsymbol{X}^s)\cdot\boldsymbol{v}+(\mathbb{X}^b+\mathbb{X}^s)\cdot\dot{\mathrm{O}}\}dA, \tag{23}$$

where $\boldsymbol{X}$, $\mathbb{X}$, and $\boldsymbol{X}^b$, $\mathbb{X}^b$ are the generalized internal forces in the body and on its boundary, respectively. $\mathbb{X}$ and $\mathbb{X}^b$ are nth-rank tensors, while $\boldsymbol{X}$ and $\boldsymbol{X}^b$ are vectors in the three-dimensional space. In particular,

$$\boldsymbol{X}=\rho(\dot{\boldsymbol{v}}-\boldsymbol{f})-\boldsymbol{\nabla}(W-\rho^2\sigma')+\mathrm{div}\left(\boldsymbol{\nabla}\mathrm{O}\odot\frac{\partial W}{\partial\boldsymbol{\nabla}\mathrm{O}}\right) \tag{24}$$

$$\mathbb{X}=\rho\left(\mathbb{M}+\frac{\partial\chi}{\partial\mathrm{O}}\right)+\frac{\partial W}{\partial\mathrm{O}}-\mathrm{div}\frac{\partial W}{\partial\boldsymbol{\nabla}\mathrm{O}} \tag{25}$$

and

$$\boldsymbol{X}^b=(W-\rho^2\sigma')\boldsymbol{\nu}-\left(\boldsymbol{\nabla}\mathrm{O}\odot\frac{\partial W}{\partial\boldsymbol{\nabla}\mathrm{O}}\right)\boldsymbol{\nu} \tag{26}$$

$$\mathbb{X}^b=\frac{\partial W}{\partial\boldsymbol{\nabla}\mathrm{O}}\boldsymbol{\nu}, \tag{27}$$

where $\boldsymbol{\nu}$ is the outer unit normal to $\partial\mathcal{B}$ and

$$\left(\boldsymbol{\nabla}\mathrm{O}\odot\frac{\partial W}{\partial\boldsymbol{\nabla}\mathrm{O}}\right)_{ij}:=O_{I,i}\frac{\partial W}{\partial O_{I,j}}. \tag{28}$$

This term shows how, because of Eq. (22), the elastic energy contributes to the generalized force $\boldsymbol{X}$ conjugated to $\boldsymbol{v}$. It will become apparent in Sec. III C how Eq. (28) can be interpreted as an elastic stress.

It should be noted that when the velocity field $\boldsymbol{v}$ is subject to a possibly differential constraint, both $\boldsymbol{X}$ and $\boldsymbol{X}^b$ may not be uniquely determined by Eq. (23) and additional terms may show up in Eqs. (24) and (27), see Sec. IV.

The special constrained variation of the total power defined in the preceding section here becomes

$$\delta(\dot{\mathcal{F}}+\mathcal{W}^s)=\int_{\mathcal{B}}\{\boldsymbol{X}\cdot\delta\boldsymbol{v}+\mathbb{X}\cdot\delta\dot{\mathrm{O}}\}dV+\int_{\partial\mathcal{B}}\{(\boldsymbol{X}^b+\boldsymbol{X}^s)\cdot\delta\boldsymbol{v}+(\mathbb{X}^b+\mathbb{X}^s)\cdot\delta\dot{\mathrm{O}}\}dA. \tag{29}$$

B. Dissipation

In the present setting $\mathcal{R}$ is indeed a functional invariant under all changes of frame (14):

$$\mathcal{R}=\int_{\mathcal{B}}RdV.$$

For any analytic dissipation function R, this requirement amounts to demand that R be the sum of invariant homogeneous terms. Thus we can assume that R is a function bilinear in $\hat{\mathbb{O}}$ and $\mathbf{D}$:

$$R = R(\mathbb{O}, \hat{\mathbb{O}}, \mathbf{D}).$$

The variation of the dissipation function here takes the form

$$\delta\mathcal{R} = \int_{\mathcal{B}} \left\{ \frac{\partial R}{\partial \dot{\mathbb{O}}} \cdot \delta\dot{\mathbb{O}} + \frac{\partial R}{\partial \nabla \boldsymbol{v}} \cdot \nabla(\delta \boldsymbol{v}) \right\} dV, \tag{30}$$

since $\delta(\nabla \boldsymbol{v}) = \nabla(\delta \boldsymbol{v})$. An integration by parts then changes Eq. (30) into

$$\delta\mathcal{R} = \int_{\mathcal{B}} \left\{ \frac{\partial R}{\partial \dot{\mathbb{O}}} \cdot \delta\dot{\mathbb{O}} - \operatorname{div}\left(\frac{\partial R}{\partial \nabla \boldsymbol{v}} \right) \cdot \delta \boldsymbol{v} \right\} dV + \int_{\partial\mathcal{B}} \left(\frac{\partial R}{\partial \nabla \boldsymbol{v}} \boldsymbol{\nu} \right) \cdot \delta \boldsymbol{v}\, dA. \tag{31}$$

Moreover, by the chain rule

$$\frac{\partial R}{\partial \dot{\mathbb{O}}} = \frac{\partial R}{\partial \hat{\mathbb{O}}} \circ \frac{\partial \hat{\mathbb{O}}}{\partial \dot{\mathbb{O}}} + \frac{\partial R}{\partial \mathbf{D}} \circ \frac{\partial \mathbf{D}}{\partial \dot{\mathbb{O}}} = \frac{\partial R}{\partial \hat{\mathbb{O}}} \tag{32}$$

and

$$\frac{\partial R}{\partial \nabla \boldsymbol{v}} = \frac{\partial R}{\partial \hat{\mathbb{O}}} \circ \frac{\partial \hat{\mathbb{O}}}{\partial \nabla \boldsymbol{v}} + \frac{\partial R}{\partial \mathbf{D}} \circ \frac{\partial \mathbf{D}}{\partial \nabla \boldsymbol{v}} = \frac{\partial R}{\partial \hat{\mathbb{O}}} \circ \frac{\partial \hat{\mathbb{O}}}{\partial \nabla \boldsymbol{v}} + \frac{\partial R}{\partial \mathbf{D}}. \tag{33}$$

Here the symbol $\circ$ denotes composition; for example, $([\partial R/\partial \hat{\mathbb{O}}] \circ [\partial \hat{\mathbb{O}}/\partial \dot{\mathbb{O}}])_I = [\partial R/\partial \hat{O}_J][\partial \hat{O}_J/\partial \dot{O}_I]$. Combining these equations with Eqs. (29) and (31), we arrive at the generalized form of Eq. (4) valid for a dissipative ordered fluid:

$$\begin{cases} \boldsymbol{X} - \operatorname{div}\left(\dfrac{\partial R}{\partial \hat{\mathbb{O}}} \circ \dfrac{\partial \hat{\mathbb{O}}}{\partial \nabla \boldsymbol{v}} + \dfrac{\partial R}{\partial \mathbf{D}} \right) = \boldsymbol{0} & \text{(34a)} \\ \qquad\qquad \text{in } \mathcal{B}, \\ \mathbb{X} + \dfrac{\partial R}{\partial \hat{\mathbb{O}}} = 0 & \text{(34b)} \end{cases}$$

and

$$\begin{cases} \boldsymbol{X}^b + \boldsymbol{X}^s + \left(\dfrac{\partial R}{\partial \hat{\mathbb{O}}} \circ \dfrac{\partial \hat{\mathbb{O}}}{\partial \nabla \boldsymbol{v}} + \dfrac{\partial R}{\partial \mathbf{D}} \right) \boldsymbol{\nu} = \boldsymbol{0} & \text{(35a)} \\ \qquad\qquad \text{on } \partial\mathcal{B}, \\ \mathbb{X}^b + \mathbb{X}^s = 0 & \text{(35b)} \end{cases}$$

In particular, the boundary equations (35) deserve a comment. When the region $\mathcal{B}$ is not free to change in time, all admissible $\delta \boldsymbol{v}$ vanish on $\partial\mathcal{B}$, and so Eq. (35a) would not properly follow from our reasoning; however, it can still be regarded as valid, provided $\boldsymbol{X}^s$ is interpreted as a *reactive* generalized force exerted by the boundary. A similar conclusion applies to Eq. (35b) and the generalized force $\mathbb{X}^s$, when $\mathbb{O}$ is prescribed on $\partial\mathcal{B}$.

Finally, it should be noticed that in arriving at Eqs. (34) and (35), we have set equal to unity the Lagrange multiplier playing here the role of λ in Sec. II. That this is indeed justified follows from Euler's theorem on homogeneous functions, by which

$$\frac{\partial R}{\partial \hat{\mathbb{O}}} \cdot \hat{\mathbb{O}} + \frac{\partial R}{\partial \mathbf{D}} \cdot \mathbf{D} = 2R, \tag{36}$$

and the linearity of the relation between the pairs $(\hat{\mathbb{O}}, \mathbf{D})$ and $(\dot{\mathbb{O}}, \nabla \boldsymbol{v})$, which together with Eq. (36) ensures that

$$\frac{\partial R}{\partial \dot{\mathbb{O}}} \cdot \dot{\mathbb{O}} + \frac{\partial R}{\partial \nabla \boldsymbol{v}} \cdot \nabla \boldsymbol{v} = 2R.$$

C. Classical balances

Equations (34) and (35) together with Eqs. (24)–(27) are the basic equations of this theory; in particular, use of Eqs. (24) and (25) in Eq. (34) yields the complete evolution equations for the body. Classically this role is played by the balance equations for linear and angular momenta. Though in the present setting it would be illusory to derive from these balances the evolution of complex microstructures such as the one described by a tensor of arbitrary rank, it remains crucial to ascertain that the evolution predicted by this theory does not violate the classical balance equations. Here we show how these equations can indeed be recognized as valid.

The balance of linear momentum requires that

$$\frac{d}{dt} \int_{\mathcal{C}} \rho \boldsymbol{v}\, dV = \int_{\mathcal{C}} \rho \boldsymbol{f}\, dV + \int_{\partial\mathcal{C}} \boldsymbol{t}\, dA \tag{37}$$

for any sub-body $\mathcal{C}$, where $\boldsymbol{f}$ is the body force per unit mass and $\boldsymbol{t}$ is the contact force per unit area. For unstructured continua, only the torques of the same forces as in Eq. (37) enter the balance of angular momentum. When, however, there is a microstructure connected with an internal rotation of the material element, additional couples in the form of body and surface moments must be accounted for. The general form of the balance of angular momentum is then

$$\frac{d}{dt} \int_{\mathcal{C}} \rho(\boldsymbol{m} + \boldsymbol{x} \times \boldsymbol{v})\, dV = \int_{\mathcal{C}} \rho(\boldsymbol{x} \times \boldsymbol{f} + \boldsymbol{k})\, dV + \int_{\partial\mathcal{C}} (\boldsymbol{x} \times \boldsymbol{t} + \boldsymbol{l})\, dA,$$

where $\boldsymbol{x}$ is the position vector, $\rho \boldsymbol{m}$ is the intrinsic angular momentum, $\boldsymbol{k}$ the body moment per unit mass, and $\boldsymbol{l}$ the surface contact moment per unit area.

When $\boldsymbol{t}$ and $\boldsymbol{l}$ at a given point are assumed to depend only on the local surface normal $\boldsymbol{\nu}$, by Cauchy's tetrahedron argument one can show that they can be expressed in terms of a stress tensor $\mathbf{T}$ and a couple stress tensor $\mathbf{L}$ according to

$$\boldsymbol{t}=\mathbf{T}\boldsymbol{\nu}, \quad \boldsymbol{l}=\mathbf{L}\boldsymbol{\nu}. \tag{38}$$

Then, by use of the conservation of mass (18), it is possible to write the classical balance equations in point form as

$$\rho\dot{\boldsymbol{v}}=\rho\boldsymbol{f}+\operatorname{div}\mathbf{T} \tag{39}$$

and

$$\rho\dot{\boldsymbol{m}}=\rho\boldsymbol{k}-\boldsymbol{\tau}+\operatorname{div}\mathbf{L}, \tag{40}$$

where $\boldsymbol{\tau}$ is associated with the skew symmetric part of $\mathbf{T}$ by $\tau_i=\epsilon_{ijk}T_{jk}$, with ϵ_{ijk} the components of Ricci's alternator. In the absence of internal rotational degrees of freedom $\dot{\boldsymbol{m}}$, $\boldsymbol{k}$, and $\mathbf{L}$ vanish and Eq. (40) reduces to the usual requirement that the stress tensor be symmetric.

Using the generalized force (24) in the equation of motion (34a), one finds that this latter takes the form (39) when the stress tensor is chosen to be

$$\mathbf{T}=(W-\rho^2\sigma')\mathbf{I}-\boldsymbol{\nabla}\mathbb{O}\odot\frac{\partial W}{\partial\boldsymbol{\nabla}\mathbb{O}}+\frac{\partial R}{\partial\hat{\mathbb{O}}}\circ\frac{\partial\hat{\mathbb{O}}}{\partial\boldsymbol{\nabla}\boldsymbol{v}}+\frac{\partial R}{\partial\mathbf{D}}, \tag{41}$$

where $\mathbf{I}$ is the identity tensor. With this choice for the stress, it follows from Eqs. (26) and (35a) that the traction on $\partial\mathcal{B}$ is balanced by the surface force $\boldsymbol{X}^s$; accordingly, it would vanish on a free surface.

To make the balance of angular momentum explicit, we enforce the requirement that the elastic energy density W be invariant under change of frame. This can be written as

$$W(O_I,O_{I,j})=W\left(O_J\prod_{m=1}^{n}Q_{I_mJ_m},O_{J,k}Q_{jk}\prod_{m=1}^{n}Q_{I_mJ_m}\right),$$

where $\mathbf{Q}$ is an arbitrary rotation. Using essentially the same arguments as in [3], one finds that this leads to

$$\epsilon_{ijk}\left[\sum_{m=1}^{n}\left(\frac{\partial W}{\partial O_{I^j_m}}O_{I^k_m}+\frac{\partial W}{\partial O_{I^j_m,l}}O_{I^k_m,l}\right)+\frac{\partial W}{\partial O_{I,j}}O_{I,k}\right]=0. \tag{42}$$

Introducing a generalized vector-valued product of two tensors of the same rank, defined by

$$(\mathbb{A}\times\mathbb{B})_i:=\epsilon_{ijk}\sum_{p=1}^{n}A_{I^j_p}B_{I^k_p},$$

Eq. (42) can also be written in compact form as

$$\mathbb{O}\times\frac{\partial W}{\partial\mathbb{O}}+\boldsymbol{\nabla}\mathbb{O}\times\frac{\partial W}{\partial\boldsymbol{\nabla}\mathbb{O}}=\boldsymbol{0}.$$

In a similar way, by requiring the kinetic energy of the microstructure $\boldsymbol{\kappa}$ to be the same in all inertial frames, we obtain

$$\mathbb{O}\times\frac{\partial\boldsymbol{\kappa}}{\partial\mathbb{O}}+\dot{\mathbb{O}}\times\frac{\partial\boldsymbol{\kappa}}{\partial\dot{\mathbb{O}}}=\boldsymbol{0}. \tag{43}$$

We are now in a position to give $\boldsymbol{\tau}$ an alternative form. Starting from the stress (41), we find

$$\tau_i=\epsilon_{ijk}\left(\frac{\partial R}{\partial\hat{O}_I}\frac{\partial\hat{O}_I}{\partial v_{j,k}}+\frac{\partial W}{\partial O_{I,j}}O_{I,k}\right), \tag{44}$$

where use has also been made of the identity $\epsilon_{ijk}A_{jk}=-\epsilon_{ijk}A_{kj}$. By Eqs. (34b) and (16), the first term on the right-hand side of Eq. (44) can be written as

$$\epsilon_{ijk}\frac{\partial R}{\partial\hat{O}_I}\frac{\partial\hat{O}_I}{\partial v_{j,k}}=\epsilon_{ijk}X_I\sum_{p=1}^{n}\delta_{jI_p}O_{I^k_p}=\epsilon_{ijk}\sum_{p=1}^{n}X_{I^j_p}O_{I^k_p},$$

where X_I are the components of $\mathbb{X}$. Thus, upon inserting Eq. (25), Eq. (44) becomes

$$\begin{aligned}\tau_i=\epsilon_{ijk}\Bigg\{&\rho\sum_{p=1}^{n}\left(M_{I^j_p}+\frac{\partial\chi}{\partial O_{I^j_p}}\right)O_{I^k_p}+\sum_{p=1}^{n}\Bigg[\frac{\partial W}{\partial O_{I^j_p}}\\&-\left(\frac{\partial W}{\partial O_{I^j_p,m}}\right)_{,m}\Bigg]O_{I^k_p}+\frac{\partial W}{\partial O_{I,j}}O_{I,k}\Bigg\}\\=\epsilon_{ijk}\rho&\sum_{p=1}^{n}\left(M_{I^j_p}+\frac{\partial\chi}{\partial O_{I^j_p}}\right)O_{I^k_p}\\&-\left(\epsilon_{ijk}\sum_{p=1}^{n}\frac{\partial W}{\partial O_{I^j_p,m}}O_{I^k_p}\right)_{,m},\end{aligned} \tag{45}$$

where the second equation follows from the identity (42).

The balance of angular momentum (40) is indeed satisfied, if we can set

$$\dot{\boldsymbol{m}}=\mathbb{O}\times\mathbb{M}, \tag{46}$$

provided we further interpret $\boldsymbol{k}$ and $\mathbf{L}$ as follows:

$$\boldsymbol{k}=-\mathbb{O}\times\frac{\partial\chi}{\partial\mathbb{O}} \tag{47}$$

and

$$L_{ij}=\epsilon_{ikl}\sum_{p=1}^{n}O_{I^k_p}\frac{\partial W}{\partial O_{I^l_p,j}}. \tag{48}$$

Actually, by Eqs. (20) and (43), Eq. (46) properly defines $\boldsymbol{m}$ as

$$\boldsymbol{m}=\mathbb{O}\times\frac{\partial\boldsymbol{\kappa}}{\partial\dot{\mathbb{O}}}. \tag{49}$$

Moreover, it follows from Eqs. (48) and (38) that

$$\boldsymbol{l}=\mathbb{O}\times\left(\frac{\partial W}{\boldsymbol{\nabla}\mathbb{O}}\boldsymbol{\nu}\right). \tag{50}$$

It is clear from Eq. (50) that the couple stress depends only on the elastic energy. The absence of any viscous contribution to the couple stress is a consequence of $\boldsymbol{\nabla}\dot{\mathbb{O}}$ being excluded from the dissipation (cf. [30] for an analogous result in a restricted setting).

IV. UNIAXIAL NEMATICS

In this section we make specific Eqs. (34) and (35) for a special family of anisotropic fluids, the uniaxial nematic liquid crystals. In the case where the scalar order parameter is constant, the dynamical equations for these materials have long been established: they were obtained as balance equations for linear and angular momenta, the latter also including the microstructural contributions [3–5]. The dynamics of uniaxial nematics with variable order was treated much later by Ericksen [6], who posited an additional balance equation for the scalar order parameter.

Our perspective here is different; the fact that for both these theories we shall arrive at the same evolution equations from an independent principle shows that all classical nematodynamics falls within the range of validity of this principle. Furthermore, it indicates that even when no guidance is gained by analogy to the balance laws of classical continuum mechanics this principle is still able to establish the basic equations of the theory. This is especially important for nematics with tensorial order [31]. Moreover, we shall illustrate here by example how to overcome the difficulties that arise when constraints are prescribed on the order tensor and the velocity field.

We proceed in two steps. First we treat in Sec. IV A the classical case with constant scalar order. We then extend these results in Sec. IV B to account also for a variable scalar order.

A. Constant scalar order parameter

A nematic liquid crystal is a fluid consisting of effectively uniaxial molecules that exhibit the tendency to align their long axes in a common direction. It is commonly described by a unit vector field $\boldsymbol{n}$, the nematic director, which indicates the local average orientation (see [32–34] for the origins of the equilibrium theory).

Most processes connected with the reorientation of the director are slow compared with the frequency of sound waves. It is then sufficient to consider the nematic fluid as incompressible. The mass density ρ is then a constant, and the divergence of the velocity field $\boldsymbol{v}$ must vanish to make the mass continuity equation satisfied. This amounts to saying that the velocity gradient $\boldsymbol{\nabla v}$ is traceless. We neglect the energy connected with the director rotation and write the total energy as

$$\mathcal{F}=\int_{\mathcal{B}}[\tfrac{1}{2}\rho\boldsymbol{v}^2+W(\boldsymbol{n},\boldsymbol{\nabla n})]dV,$$

where all external actions have been omitted for simplicity.

Our first objective is to decompose the power $\dot{\mathcal{F}}$ into conjugated velocities and forces. We choose as velocities $\boldsymbol{v}$ and the material time derivative of the director $\dot{\boldsymbol{n}}$. Here, again with the aid of Eqs. (13) and (22), Eq. (19) becomes

$$\dot{\mathcal{F}}=\int_{\mathcal{B}}\left\{\rho\dot{\boldsymbol{v}}\cdot\boldsymbol{v}+\left(\frac{\partial W}{\partial\boldsymbol{n}}-\mathrm{div}\frac{\partial W}{\partial\boldsymbol{\nabla n}}\right)\cdot\dot{\boldsymbol{n}}-\left((\boldsymbol{\nabla n})^T\frac{\partial W}{\partial\boldsymbol{\nabla n}}\right)\cdot\boldsymbol{\nabla v}\right\}dV+\int_{\partial\mathcal{B}}\left(\frac{\partial W}{\partial\boldsymbol{\nabla n}}\boldsymbol{\nu}\right)\cdot\dot{\boldsymbol{n}}dA. \tag{51}$$

Since $\dot{\boldsymbol{n}}$ is orthogonal to $\boldsymbol{n}$ and $\boldsymbol{\nabla v}$ is traceless, the power $\dot{\mathcal{F}}$ remains unchanged whenever the integrands in Eq. (51) are altered as follows:

$$\dot{\mathcal{F}}=\int_{\mathcal{B}}\left\{\rho\dot{\boldsymbol{v}}\cdot\boldsymbol{v}+\left(\frac{\partial W}{\partial\boldsymbol{n}}-\mathrm{div}\frac{\partial W}{\partial\boldsymbol{\nabla n}}+\mu\boldsymbol{n}\right)\cdot\dot{\boldsymbol{n}}-\left((\boldsymbol{\nabla n})^T\frac{\partial W}{\partial\boldsymbol{\nabla n}}+p\mathbf{I}\right)\cdot\boldsymbol{\nabla v}\right\}dV+\int_{\partial\mathcal{B}}\left(\frac{\partial W}{\partial\boldsymbol{\nabla n}}\boldsymbol{\nu}+\mu_b\boldsymbol{n}\right)\cdot\dot{\boldsymbol{n}}dA, \tag{52}$$

where μ, μ_b, and p are arbitrary scalar fields. An integration by parts in Eq. (52) then allows to identify the generalized forces

$$\boldsymbol{X}=\rho\dot{\boldsymbol{v}}+\mathrm{div}\left((\boldsymbol{\nabla n})^T\frac{\partial W}{\partial\boldsymbol{\nabla n}}+p\mathbf{I}\right), \tag{53}$$

$$\mathbb{X}=\frac{\partial W}{\partial\boldsymbol{n}}-\mathrm{div}\frac{\partial W}{\partial\boldsymbol{\nabla n}}+\mu\boldsymbol{n}, \tag{54}$$

$$\boldsymbol{X}^b=\left((\boldsymbol{\nabla n})^T\frac{\partial W}{\partial\boldsymbol{\nabla n}}+p\mathbf{I}\right)\boldsymbol{\nu}, \tag{55}$$

$$\mathbb{X}^b=\frac{\partial W}{\partial\boldsymbol{\nabla n}}\boldsymbol{\nu}+\mu_b\boldsymbol{n}, \tag{56}$$

where clearly μ, μ_b, and p appear as Lagrange multipliers corresponding to the constraints that both $\mathbb{X}$ and $\mathbb{X}^b$ be orthogonal to $\boldsymbol{n}$, and $\boldsymbol{v}$ be a solenoidal field.

Following the general format set forth in Sec. III, we assume that the dissipation density is a function $R=R(\boldsymbol{n},\mathring{\boldsymbol{n}},\mathbf{D})$ bilinear in the symmetric part $\mathbf{D}$ of $\boldsymbol{\nabla v}$ and the corotational time derivative $\mathring{\boldsymbol{n}}$ of the director. The latter is represented as

$$\mathring{\boldsymbol{n}}=\dot{\boldsymbol{n}}-\boldsymbol{\omega}\times\boldsymbol{n},$$

where $\boldsymbol{\omega}=\frac{1}{2}\,\mathrm{curl}\,\boldsymbol{v}$ is the axial vector of the skew-symmetric part $\mathbf{W}$ of $\boldsymbol{\nabla v}$, so that $\mathring{\boldsymbol{n}}=\dot{\boldsymbol{n}}-\mathbf{W}\boldsymbol{n}$.

Equation (36) here reads as

$$\frac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}}\cdot\overset{\circ}{\boldsymbol{n}}+\frac{\partial R}{\partial \mathbf{D}}\cdot\mathbf{D}=2R. \tag{57}$$

Similarly, Eqs. (32) and (33) become

$$\frac{\partial R}{\partial \dot{\boldsymbol{n}}}=\frac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}} \tag{58}$$

and

$$\frac{\partial R}{\partial \boldsymbol{\nabla v}}=\frac{1}{2}\left(\boldsymbol{n}\otimes\frac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}}-\frac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}}\otimes\boldsymbol{n}\right)+\frac{\partial R}{\partial \mathbf{D}}. \tag{59}$$

By combining Eqs. (53)–(56) with (58) and (59), we can now write Eqs. (34a) and (35a) in the following form

$$\begin{cases}\rho\dot{\boldsymbol{v}}=\operatorname{div}\mathbf{T} & \text{(60a)}\\ \dfrac{\partial W}{\partial \boldsymbol{n}}-\operatorname{div}\dfrac{\partial W}{\partial \boldsymbol{\nabla n}}+\dfrac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}}+\mu\boldsymbol{n}=\boldsymbol{0} & \text{(60b)}\end{cases}\quad \text{in}\quad \mathcal{B},$$

and

$$\begin{cases}\mathbf{T}\boldsymbol{\nu}+\boldsymbol{X}^s=\boldsymbol{0} & \text{(61a)}\\ \dfrac{\partial W}{\partial \boldsymbol{\nabla n}}\boldsymbol{\nu}+\mu_b\boldsymbol{n}+\mathbb{X}^s=\boldsymbol{0} & \text{(61b)}\end{cases}\quad \text{on}\quad \partial\mathcal{B},$$

with the stress

$$\mathbf{T}=-p\mathbf{I}-(\boldsymbol{\nabla n})^T\frac{\partial W}{\partial \boldsymbol{\nabla n}}+\frac{1}{2}\left(\boldsymbol{n}\otimes\frac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}}-\frac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}}\otimes\boldsymbol{n}\right)+\frac{\partial R}{\partial \mathbf{D}}. \tag{62}$$

It is clear from Eq. (62) that the extra-stress $\mathbf{T}+p\mathbf{I}$ can be decomposed into the sum of an *elastic* stress

$$\mathbf{T}^{(\mathrm{e})}:=-(\boldsymbol{\nabla n})^T\frac{\partial W}{\partial \boldsymbol{\nabla n}}$$

and a *viscous* stress

$$\mathbf{T}^{(\mathrm{v})}:=\frac{1}{2}\left(\boldsymbol{n}\otimes\frac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}}-\frac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}}\otimes\boldsymbol{n}\right)+\frac{\partial R}{\partial \mathbf{D}}.$$

The axial vector associated with the skew-symmetric part of $\mathbf{T}^{(\mathrm{v})}$ is $-\boldsymbol{n}\times(\partial R/\partial\overset{\circ}{\boldsymbol{n}})$, with the meaning of a viscous torque on $\boldsymbol{n}$; hence Eq. (60b), once written in the equivalent form

$$\boldsymbol{n}\times\left(\operatorname{div}\frac{\partial W}{\partial \boldsymbol{\nabla n}}-\frac{\partial W}{\partial \boldsymbol{n}}-\frac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}}\right)=\boldsymbol{0},$$

can be interpreted as a balance of torques acting on the director. A similar interpretation can also be given for Eq. (61b). Moreover, according to Eq. (48) the components of the couple stress tensor read as

$$L_{ij}=\epsilon_{ikl}n_k\frac{\partial W}{\partial n_{l,j}}.$$

We have thus recovered in our setting the classical theory for nematodynamics (cf. especially Eqs. (2.4) and (5.6) of [30]).

The most general dissipation function bilinear in $\overset{\circ}{\boldsymbol{n}}$ and $\mathbf{D}$ can be found by considering all possible scalar invariants that can be built from these quantities and the director $\boldsymbol{n}$. This function can be written as

$$R=\tfrac{1}{2}\gamma_1\overset{\circ}{\boldsymbol{n}}^2+\gamma_2\overset{\circ}{\boldsymbol{n}}\cdot\mathbf{D}\boldsymbol{n}+\tfrac{1}{2}\gamma_3(\mathbf{D}\boldsymbol{n})^2+\tfrac{1}{2}\gamma_4\operatorname{tr}\mathbf{D}^2+\tfrac{1}{2}\gamma_5(\boldsymbol{n}\cdot\mathbf{D}\boldsymbol{n})^2, \tag{63}$$

where the γ's are constants. It readily follows that

$$\frac{\partial R}{\partial \mathbf{D}}=\tfrac{1}{2}\gamma_2(\overset{\circ}{\boldsymbol{n}}\otimes\boldsymbol{n}+\boldsymbol{n}\otimes\overset{\circ}{\boldsymbol{n}})+\tfrac{1}{2}\gamma_3(\mathbf{D}\boldsymbol{n}\otimes\boldsymbol{n}+\boldsymbol{n}\otimes\mathbf{D}\boldsymbol{n})+\gamma_4\mathbf{D}+\gamma_5(\boldsymbol{n}\cdot\mathbf{D}\boldsymbol{n})\boldsymbol{n}\otimes\boldsymbol{n}$$

and

$$\frac{\partial R}{\partial \overset{\circ}{\boldsymbol{n}}}=\gamma_1\overset{\circ}{\boldsymbol{n}}+\gamma_2\mathbf{D}\boldsymbol{n}.$$

The form of the viscous stress commonly used is

$$\mathbf{T}^{(v)}=\alpha_1(\boldsymbol{n}\cdot\mathbf{D}\boldsymbol{n})\boldsymbol{n}\otimes\boldsymbol{n}+\alpha_2\overset{\circ}{\boldsymbol{n}}\otimes\boldsymbol{n}+\alpha_3\boldsymbol{n}\otimes\overset{\circ}{\boldsymbol{n}}+\alpha_4\mathbf{D}+\alpha_5\mathbf{D}\boldsymbol{n}\otimes\boldsymbol{n}+\alpha_6\boldsymbol{n}\otimes\mathbf{D}\boldsymbol{n},$$

where the α's are Leslie's coefficients [cf. [30], Eq. (4.6)]. This expression is the same as ours, provided that

$$\alpha_1=\gamma_5,\quad \alpha_2=\tfrac{1}{2}(\gamma_2-\gamma_1),\quad \alpha_3=\tfrac{1}{2}(\gamma_2+\gamma_1),$$
$$\alpha_4=\gamma_4,\quad \alpha_5=\tfrac{1}{2}(\gamma_3-\gamma_2),\quad \alpha_6=\tfrac{1}{2}(\gamma_3+\gamma_2),$$

where it follows that $\alpha_6-\alpha_5=\alpha_2+\alpha_3$, known as the Onsager-Parodi relation. This relation is automatically satisfied because the generalized viscous forces derive from a potential R. Here indeed Onsager's principle reduces to the symmetry in the mixed second derivatives of R.

Finally, it is worth remarking that using a codeformational time derivative $\hat{\boldsymbol{n}}=\overset{\circ}{\boldsymbol{n}}+\alpha\mathbf{D}\boldsymbol{n}$ rather than $\overset{\circ}{\boldsymbol{n}}$ in constructing the dissipation function would in general result in ordering differently the same terms in Eq. (63); in particular, whenever both γ_2 and γ_3 do not vanish, the theory would not be formally affected.

B. Variable scalar order parameter

The local degree of order of a uniaxial nematic liquid crystal can be measured by the Maier-Saupe order parameter S, which is given by

$$S=\langle P_2(\boldsymbol{n}\cdot\boldsymbol{u})\rangle, \tag{64}$$

where the brackets $\langle\cdots\rangle$ indicate a local orientational average over the molecules and P_2 is the second Legendre polynomial in $\boldsymbol{n}\cdot\boldsymbol{u}$, the cosine of the angle between the molecular

figure axis $\boldsymbol{u}$ and the nematic director $\boldsymbol{n}$. S can take values between $-1/2$ and 1. To describe the average orientation along with the scalar order, it is convenient to employ the uniaxial second-rank alignment tensor

$$\mathbf{a}=S(\boldsymbol{n}\otimes\boldsymbol{n}-\tfrac{1}{3}\mathbf{I}), \tag{65}$$

which also reflects the *nematic symmetry*, i.e., the physical equivalence of $\boldsymbol{n}$ and $-\boldsymbol{n}$. By use of Eq. (65), a theory for uniaxial nematics with variable order is obtained naturally as a special case of a theory for the full second-rank alignment tensor [31]. However, here we prefer to treat S and $\boldsymbol{n}$ as two independent variables. In this way we can profit from the results of the preceding subsection.

The energy connected with the order is now a function $W=W(S,\boldsymbol{\nabla}S,\boldsymbol{n},\boldsymbol{\nabla}\boldsymbol{n})$, and it will in general contain not only elastic terms, but also a Landau-deGennes potential in S. Using the same method illustrated above, one finds an additional term in the generalized force (53), which here becomes

$$\boldsymbol{X}=\rho\dot{\boldsymbol{v}}+\mathrm{div}\left((\boldsymbol{\nabla}\boldsymbol{n})^{T}\frac{\partial W}{\partial\boldsymbol{\nabla}\boldsymbol{n}}+\boldsymbol{\nabla}S\otimes\frac{\partial W}{\partial\boldsymbol{\nabla}S}+p\mathbf{I}\right). \tag{66}$$

Equation (54) remains unchanged, and a third generalized force conjugated to $\dot{S}$ is found as

$$X^{(S)}=\frac{\partial W}{\partial S}-\mathrm{div}\frac{\partial W}{\partial\boldsymbol{\nabla}S}, \tag{67}$$

which enters the balance equation

$$X^{(S)}+\frac{\partial R}{\partial\dot{S}}=0. \tag{68}$$

Since S is scalar, its material time derivative $\dot{S}$ is frame-indifferent, and we can write the dissipation function as $R=R(\boldsymbol{n},\mathring{\boldsymbol{n}},S,\dot{S},\mathbf{D})$. The most general form this can take is

$$R=\beta_1\dot{S}\boldsymbol{n}\cdot\mathbf{D}\boldsymbol{n}+\tfrac{1}{2}\beta_2\dot{S}^2 \tag{69}$$

$$+\tfrac{1}{2}\gamma_1\mathring{\boldsymbol{n}}^2+\gamma_2\mathring{\boldsymbol{n}}\cdot\mathbf{D}\boldsymbol{n}+\tfrac{1}{2}\gamma_3(\mathbf{D}\boldsymbol{n})^2+\tfrac{1}{2}\gamma_4\,\mathrm{tr}\,\mathbf{D}^2+\tfrac{1}{2}\gamma_5(\boldsymbol{n}\cdot\mathbf{D}\boldsymbol{n})^2, \tag{70}$$

where now all β's and γ's are arbitrary functions of S.

It then follows that the equations of motion still hold in the form (60), where the stress is given by the tensor in Eq. (62) plus the one related to the scalar order:

$$\mathbf{T}^{(S)}=-\boldsymbol{\nabla}S\otimes\frac{\partial W}{\partial\boldsymbol{\nabla}S}+\beta_1\dot{S}\boldsymbol{n}\otimes\boldsymbol{n}. \tag{71}$$

Furthermore, the additional equation (68) becomes

$$\frac{\partial W}{\partial S}-\mathrm{div}\frac{\partial W}{\partial\boldsymbol{\nabla}S}+\beta_1\boldsymbol{n}\cdot\mathbf{D}\boldsymbol{n}+\beta_2\dot{S}=0. \tag{72}$$

Apart from the microinertia, which we have neglected here, the evolution equations that we find are the same as Ericksen's [6], where again the extra Onsager relation he derived is automatically satisfied.

V. CONCLUSIONS

We adopted a variational principle to extend the classical Lagrange-Rayleigh equations of mass-point dynamics to fluids with dissipative microstructure, where the internal order is described by a tensor of arbitrary rank. In this way, starting only from the free energy and the dissipation, we arrived directly at the evolution equations for the fluid along with the appropriate boundary conditions.

We compared this theory to the classical one, where the evolution equations arise from writing balances together with constitutive assumptions. It turned out that the flow equation can always be interpreted as the balance of linear momentum, where the stress tensor derives directly from the free energy and the dissipation. Similarly, the balance of angular momentum follows from the evolution equation for the order tensor: We made use of invariance properties of both elastic and kinetic energies to identify the internal angular momentum and both body and contact couples.

While it is always possible to reconcile our approach with the classical balance equations, the reverse does not hold true. In general, the internal order has more than just the rotational degrees of freedom, and so additional balances and constitutive relations would be needed.

As a specific example, we showed how the hydrodynamic theory for uniaxial nematic liquid crystals is derived within our setting. In particular, this illustrates how special constraints can be treated. For a constant scalar order parameter, we found the stress tensor in the form used in the Ericksen-Leslie-Parodi theory. While one can reconcile in the bulk this stress with the symmetric stress of the Harvard group [1], p. 208, by adding a divergence-free term, this is not possible on the boundary because it would contradict the boundary conditions. In the more general case of variable degree of orientation we found the additional contributions to the stress and a balance equation for the scalar order parameter in the form proposed by Ericksen [6].

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