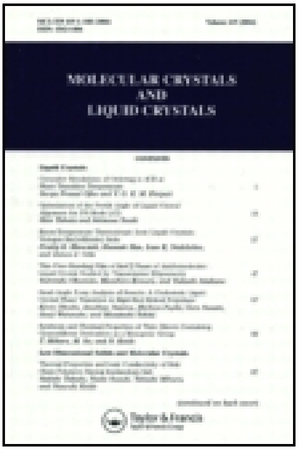

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The Dynamical Behavior of Liquid Crystals: A Continuum Description through Generalized Brackets

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The Dynamical Behavior of Liquid Crystals: A Continuum Description through Generalized Brackets

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In this paper, we systematically develop a hierarchy of constitutive equations at various levels of abstraction for describing the dynamics of incompressible liquid-crystalline systems. We also introduce a corresponding hierarchy of generalized bracket formulations. The simplest brackets, in terms of the direction vector, are capable of generating the Leslie-Ericksen (LE) theory in both the standard form of the equations (inertial) as well as the form in which the inertia associated with the rotation of the director is neglected. In parallel, a second, more-complex class of brackets is introduced, in terms of a structural tensor, which generates a theory that is more general than the LE theory, in that it can describe more-diverse phenomena, such as biaxiality and phase transitions. As particular cases, the generalized equations reduce to the LE equations or the more recent theory of Ericksen under the uniaxial approximation. Thus the collection of the governing equations of the generalized theory represents an inherently consistent set, which covers all the range from the director (LE-type) theories and the order-parameter (Doi-type) theories.

Keywords: liquid crystals, rheological theory, poisson bracket, hamiltonian formulation, tensorial parameters

1. INTRODUCTION

In the 1960's, Leslie and Ericksen[1–5] introduced a theory which describes the dynamics of liquid-crystalline systems based upon the motion of a direction unit vector, n, called the director. Though, in general, quite successful, the theory still suffered from several drawbacks. First, due to the form of the dissipation in the unit vector description, it was only applicable in the small, linear deformation rate regime. Also, the use of the unit vector to describe the orientation excludes from the problem formulation a lot of interesting physics and observed phenomena which occur in liquid crystals; for instance, biaxiality and phase transitions.[6]

In the early 1980's, Doi introduced equations for liquid crystals (rigid-rods) based upon a structural tensor, **S**, called the order-parameter tensor.[7-10] This theory also had successes; it was applicable in the non-linear flow regime and could describe the isotropic/nematic phase transition in lyotropic liquid crystals. Its drawbacks were that it could not describe spatial inhomogeneities in the orientation and has neglected inertial effects associated with the rotation of the director (it is a quasi-steady state theory).

Recently, Grmela[11] has introduced an objective reference frame Poisson bracket which can be used to generate complex constitutive equations, based upon the Hamiltonian (free energy) of a given system, and of course, the dissipation. The details of the Poisson bracket formulation can be found in References 11 and 12. Also recently, Edwards *et al.*[13,14] used an objective Poisson bracket to develop a general constitutive equation for liquid crystals, based upon a tensor structural parameter. This theory reduces to Doi's theory in the homogeneous limit, and describes not only the phase transitions, but also the spatial inhomogeneities which occur in the orientation. In addition, similar predictions for the initial stages of a spinodal decomposition from the isotropic to the nematic state are obtained[14] compared to those of Doi's extended distribution-function theory.[15] However, being derived from an objective frame Poisson bracket, the model is still incapable of accounting for inertial effects associated with sudden changes in orientation, which may be important in some applications.[6] The objective of this paper is to close this gap, and in so doing, to complete the cycle of elucidating the connections between the unit-vector and order-parameter theories for liquid-crystalline flow behavior.

The underlying idea behind this paper is to introduce a consistent set of alternate formulations for incompressible liquid-crystalline flows. In Section 2, we describe the Leslie-Ericksen (LE) theory for both an inertial and a non-inertial frame of reference. In the former, the primary system variables are the velocity vector, u, the director, n, as well as the material (substantial) time derivative of the director, $\dot{n}$. In the latter, the primary variables are just u and n. In Section 3, we present the corresponding generalized bracket formulation to the LE equations for both reference frames. This allows a consistent generalization of the LE theory in Section 4 to a theory in terms of a tensorial parameter, $\mathbf{m}$, which describes the fluid structure, for both reference frames. As already pointed out, the use of a tensorial structural parameter allows a greater variety of phenomena to be incorporated into the theory. In the fully-aligned uniaxial flow approximation, when $\mathbf{m} = nn$, we shall see that the LE equations arise as a special case of the generalized theory. In Section 5, we discuss the significance of the results of §3 and 4, as well as demonstrate the connections between the various theories described above.

Lately, Ericksen[16] and Calderer[17,18] have been using a model similar to the LE theory based upon a scalar-vector description of the orientation, i.e., by considering a scalar parameter, s, in addition to the director which describes the distribution around the preferred direction. The generalized bracket formulation can also be used to arrive at this type of approach. We relegate this discussion to Appendix A so as not to obscure the vector-tensor transition in the main body of this paper. Likewise, the scalar-vector theory can be shown to be a special case of the general tensor theory under the uniaxial approximation, $\mathbf{m} = \mathrm{s}nn + (1 - \mathrm{s})\,\delta/3$.

As a last item in the introduction, let us present Figure 1, which shows schematically the various levels of description, within the limits of continuum mechanics, for liquid-crystalline systems. The most exact methods of describing the dynamics of liquid crystals are through kinetic theory or higher-order phenomenological theories. These, however, are generally too complicated to allow solutions to the equations to be obtained, except in the simplest circumstances. The most general

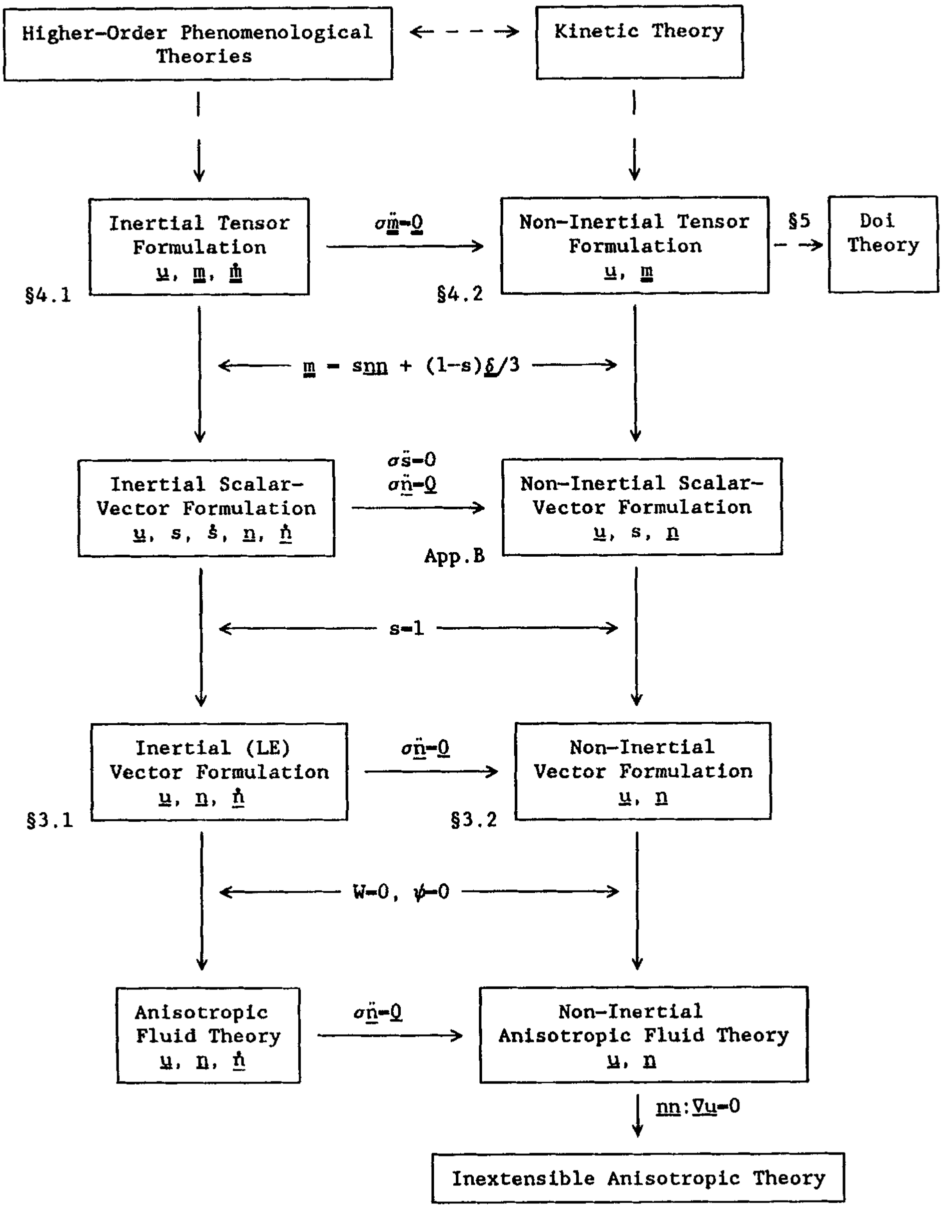

FIGURE 1 Levels of description for liquid-crystalline systems.

method of description which allows simple solutions for most interesting problems is that in terms of a single structural tensor, **m** (or $\dot{\mathbf{m}}$ and its material derivative in the inertial-frame theory). As special cases, we get all of the lower-level theories represented by the scalar-vector and vector levels in both their inertial and non-inertial forms. Of course, as we reduce the level of description, we preclude more and more physics from the ensuing development. Hopefully, the general tensor theory in terms of **m** will represent the best compromise between the higher-order (but very complicated) theories and the simple (but often oversimplified) vector descriptions.

Although the mathematics of the generalized bracket approach is straightforward, the algebra is often very tedious (especially for such complex materials as liquid crystals). It is thus more important to follow the spirit of this paper, rather than all of the minute mathematical details. The important points to recognize in this paper are that all the liquid-crystalline descriptions possess the same underlying structure (Hamiltonian structure) as all other transport phenomena. The major results of this paper, in addition to the demonstration of the Hamiltonian form of the equations, are the two sets of governing equations in terms of the structural tensor, for both inertial and non-inertial frames. Hopefully, the ensuing mathematics will not obscure the importance of these issues.

2. LESLIE-ERICKSEN THEORY

2.1 Inertial Theory

In the theory of Leslie-Ericksen[1-5] for incompressible liquid-crystalline systems, the short-range order of the system is described by the vector n, called the director, which is defined to be of unit length and, as such, subject to the constraint

$$n \cdot n = 1 \tag{2.1}$$

The states of n and $-n$ are physically indistinguishable from each other due to the invariance of the molecules under a rotation of 180 degrees.

For flowing systems, two constitutive relations describe the kinematics of the director:

$$\rho \dot{u}_\alpha = F_\alpha - p_{,\alpha} - \left(\frac{\partial W}{\partial n_{\gamma,\beta}} n_{\gamma,\alpha} \right)_{,\beta} + t_{\alpha\beta,\beta}; \tag{2.2}$$

$$\sigma \ddot{n}_\alpha = G_\alpha + \gamma n_\alpha - \frac{\partial W}{\partial n_\alpha} + \left(\frac{\partial W}{\partial n_{\alpha,\beta}} \right)_{,\beta} + g_\alpha; \tag{2.3}$$

where a superscripted dot denotes the material (substantial) derivative, i.e.,

$$\dot{a}_\alpha \equiv \frac{\partial a_\alpha}{\partial t} + u_\beta a_{\alpha,\beta}. \tag{2.4}$$

Note that the Einstein summation convention has been used, with commas denoting spatial derivatives.

Equation (2.2) reflects the law of conservation of linear momentum. In this expression, ρ is the constant density of the system, u is the velocity vector subject to the incompressibility constraint,

$$\operatorname{div} u = 0, \tag{2.5}$$

p is the pressure and F is a body force vector due to an external force field. For an external magnetic field, H, which induces in the material a magnetization, M,

$$F_\alpha = M_\beta H_{\beta,\alpha}, \tag{2.6}$$

where

$$M_\alpha = \chi_\perp H_\alpha + (\chi_\parallel - \chi_\perp) n_\beta H_\beta n_\alpha, \tag{2.7}$$

and $\chi_\perp$ and $\chi_\parallel$ are the magnetic susceptibilities perpendicular and parallel to the director, respectively.

The last two terms in Equation (2.2) represent the effects of the extra stress. The first term is due to the Ericksen stress,[1] which reflects the elastic distortion stress of the system, arising from the Frank distortion energy,[19] W, given by

$$2W = K_1(\operatorname{div} n)^2 + K_2(n \cdot \operatorname{curl} n)^2 + K_3[(n \cdot \nabla)n]^2. \tag{2.8}$$

$t_{\alpha\beta}$ is the dissipative portion of the stress, which must satisfy thermodynamic criteria. It is given as

$$t_{\alpha\beta} = \alpha_1 n_\gamma n_\varepsilon A_{\gamma\varepsilon} n_\alpha n_\beta + \alpha_2 N_\alpha n_\beta + \alpha_3 N_\beta n_\alpha + \alpha_4 A_{\alpha\beta} + \alpha_5 A_{\alpha\gamma} n_\gamma n_\beta + \alpha_6 A_{\beta\gamma} n_\gamma n_\alpha, \tag{2.9}$$

where

$$2A_{\alpha\beta} = u_{\alpha,\beta} + u_{\beta,\alpha}, \tag{2.10}$$

$$N_\alpha = \dot{n}_\alpha - \Omega_{\alpha\beta} n_\beta, \tag{2.11}$$

and

$$2\Omega_{\alpha\beta} = u_{\alpha,\beta} - u_{\beta,\alpha}. \tag{2.12}$$

The α_i must satisfy all of the thermodynamic criteria presented by Leslie,[4] and the relation of Parodi[20] (see also Appendix C):

$$\alpha_2 + \alpha_3 = \alpha_6 - \alpha_5. \tag{2.13}$$

(Later, we shall see how this relation arises through the generalized bracket formulation.)

Equation (2.3) is an angular momentum balance. In this expression, σ is an inertial constant, $\ddot{n}$ is the material derivative of $\dot{n}$, and G is a director body force resulting from the magnetic field, expressed as,

$$G_\alpha = \chi_a n_\beta H_\beta H_\alpha, \tag{2.14}$$

with χ_a being the difference in the magnetic susceptibilities. Dissipation is included in this expression through g_α, which is given as

$$g_\alpha = -\gamma_1 N_\alpha - \gamma_2 A_{\alpha\beta} n_\beta; \quad \gamma_1 = \alpha_3 - \alpha_2 \quad \text{and} \quad \gamma_2 = \alpha_6 - \alpha_5, \tag{2.15}$$

γ in Equation (2.3) insures that n remains a unit vector,

$$\gamma = -G_\beta n_\beta + \frac{\partial W}{\partial n_\beta} n_\beta - n_\beta \left(\frac{\partial W}{\partial n_{\beta,\gamma}}\right)_{,\gamma} + (\alpha_2 + \alpha_3) u_{\beta,\gamma} n_\gamma n_\beta - \sigma \dot{n}_\beta \dot{n}_\beta, \tag{2.16}$$

i.e., dotting Equation (2.3) with n using the above value of γ gives zero. Note that Equations (2.1) and (2.4) imply the additional constraint

$$\dot{n} \cdot n = 0. \tag{2.17}$$

The above system of equations form a closed set which, in principle, can be solved for arbitrary kinematics.

2.2 Non-Inertial Theory

For viscous materials, a "quasi-steady state" theory can be developed by neglecting changes in time of the material derivative of the director, i.e., using the quasi-steady state assumption:

$$\sigma \ddot{n}_\alpha = 0, \tag{2.18}$$

which can be achieved by assuming $\sigma \to 0$. In this case, we can use Equations (2.3, 10–12, 15) to solve directly for the time derivative of the director, $\dot{n}$, as

$$\dot{n}_\alpha = \frac{\alpha_2}{(\alpha_2 - \alpha_3)} u_{\alpha,\beta} n_\beta + \frac{\alpha_3}{(\alpha_2 - \alpha_3)} u_{\beta,\alpha} n_\beta - \frac{1}{(\alpha_2 - \alpha_3)} G_\alpha - \frac{1}{(\alpha_2 - \alpha_3)} \gamma n_\alpha + \frac{1}{(\alpha_2 - \alpha_3)} \left[\frac{\partial W}{\partial n_\alpha} - \left(\frac{\partial W}{\partial n_{\alpha,\beta}}\right)_{,\beta}\right], \tag{2.19}$$

where we have used the Parodi relation of Equation (2.13). Substituting this expression into Equation (2.9) results in a new equation for the stress tensor:

$$
\begin{aligned}
t''_{\alpha\beta} = {} & \beta_1 A_{\gamma\varepsilon} n_\gamma n_\varepsilon n_\alpha n_\beta + \beta_2 A_{\alpha\beta} + \beta_3 [A_{\alpha\gamma} n_\gamma n_\beta + A_{\beta\gamma} n_\gamma n_\alpha] \\
& - \frac{(\alpha_2 + \alpha_3)}{(\alpha_2 - \alpha_3)} \gamma n_\alpha n_\beta - \frac{1}{(\alpha_2 - \alpha_3)} [\alpha_2 G_\alpha n_\beta + \alpha_3 G_\beta n_\alpha] \\
& + \frac{1}{(\alpha_2 - \alpha_3)} \left[\alpha_2 \frac{\partial W}{\partial n_\alpha} n_\beta + \alpha_3 \frac{\partial W}{\partial n_\beta} n_\alpha \right] \\
& - \frac{1}{(\alpha_2 - \alpha_3)} \left[\alpha_2 \left(\frac{\partial W}{\partial n_{\alpha,\gamma}} \right)_{,\gamma} n_\beta + \alpha_3 \left(\frac{\partial W}{\partial n_{\beta,\gamma}} \right)_{,\gamma} n_\alpha \right],
\end{aligned} \tag{2.20}
$$

where

$$
\beta_1 = \alpha_1, \quad \beta_2 = \alpha_4, \quad \text{and} \quad \beta_3 = \frac{\alpha_6 \alpha_2 - \alpha_5 \alpha_3}{(\alpha_2 - \alpha_3)}. \tag{2.21}
$$

Thus we arrive at the non-inertial version of the LE theory as given by Equations (2.2, 19, 20).

If we were to set $G = 0$ and $W = 0$ (i.e., no external field nor distortion energy) in the above equations, then the equations should reduce to Ericksen's transversely isotropic fluid.[1] In this case, if we incorporate γ into the first three terms of Equation (2.20), we get the new phenomenological coefficients

$$
\beta_1^n = \alpha_1 - \frac{(\alpha_2 + \alpha_3)^2}{(\alpha_2 - \alpha_3)}, \quad \beta_2^n = \alpha_4, \quad \text{and} \quad \beta_3^n = \frac{\alpha_6 \alpha_2 - \alpha_5 \alpha_3}{(\alpha_2 - \alpha_3)}. \tag{2.22}
$$

We shall use only the parameters of Equation (2.22) in the remainder of this paper. Also note that if we impose, in addition to $G = 0$ and $W = 0$, the constraint $nn : \nabla u = 0$, then the equations of an axially-inextensible transversely isotropic linear viscous fluid are obtained. These equations have been used very recently[21,22] to provide constitutive relationships for a continuous fiber-reinforced Newtonian fluid in thermoplastic composites manufacturing processes.

3. GENERALIZED BRACKET FORMULATION IN TERMS OF VECTOR PARAMETERS

In this section, we derive the LE equations presented in the preceding section for both reference frames using the generalized bracket formulation. This exercise allows us to rewrite the LE equations in an alternate form, i.e., in *Hamiltonian form*. Once we realize the underlying structure of this system of equations, we can then generalize it in §4 to a theory in terms of tensorial structural parameters.

3.1 Inertial Theory

Let us assume that the liquid-crystalline material is described by three vector fields: the velocity, u, the director, n and the (as yet) unspecified vector, ω. Later, this parameter will be identified as the material derivative of the director (multiplied by the inertial constant σ), $\sigma\dot{n}$. We treat it temporarily as an independent parameter in order to illustrate that applying the constraint $n \cdot n = 1$ to the Poisson bracket automatically ensures that the constraint $\dot{n} \cdot n = 0$ is satisfied without imposing it explicitly.

Following References 11–13, the time evolution equations for the state variables are introduced in the generalized bracket formulation as follows. Let F, G and H be sufficiently regular functionals of u, n and ω which can be written in terms of an integral expression, such as

$$F[u, n, \omega] = \int_\Omega f(u, n, \omega)\, dV, \tag{3.1}$$

with $f(u, n, \omega)$ being an arbitrary (with suitable continuity) integrable scalar function of u, n and ω over the domain Ω. The time derivative for the arbitrary functional, F, is then expressed as

$$\frac{dF}{dt} = \int_\Omega \left(\frac{\delta F}{\delta u} \cdot \frac{\partial u}{\partial t} + \frac{\delta F}{\delta n} \cdot \frac{\partial n}{\partial t} + \frac{\delta F}{\delta \omega} \cdot \frac{\delta \omega}{\delta t} \right) dV, \tag{3.2a}$$

or,

$$\frac{dF}{dt} = \{(F, H)\}, \tag{3.2b}$$

where H is the Hamiltonian (energy) functional and $\{(.\ ,\ .)\}$ is a generalized bracket operation.

The Hamiltonian of the system is defined by the expression[2,5]

$$H[u, n, \omega] = \int_\Omega \left(\frac{1}{2} \rho u \cdot u + \frac{1}{2\sigma} \omega \cdot \omega + W + \psi_m \right) dV. \tag{3.3}$$

In Equation (3.3), the first two terms represent the translational and rotational kinetic energy, respectively. In the following the units of mass and length are so chosen so as to make the density, ρ, equal unity (for convenience). W is the Frank distortion energy,[19] given by Equation (2.8), which represents the effects of spatial variations on the director field. The last term ψ_m, includes the effects of an external magnetic field into the system of equations. It is given as

$$\psi_m \equiv -\frac{1}{2} [\chi_a (n \cdot H)^2 + \chi_\perp H \cdot H]. \tag{3.4}$$

The generalized bracket {(. , .)} is defined for two arbitrary functionals, F and G, as[12]

$$\{(F, G)\} \equiv \{F, G\} - [F, G], \tag{3.5}$$

where $\{F, G\}$ is a suitable Poisson bracket,[11,12] satisfying the antisymmetry property and the Jacobi identity, and $[F, G]$ is a dissipation bracket[12] which must be a non-negative bilinear form.

The inertial Poisson bracket for two arbitrary functionals, $F[u, \tilde{n}, \omega]$ and $G[u, \tilde{n}, \omega]$, where $\tilde{n}$ is the unconstrained direction vector (i.e., not a unit vector), can be written as

$$\begin{aligned}\{F, G\} = &- \int_\Omega u_\alpha \left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta u_\alpha} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta u_\alpha}\right) dV \\ &- \int_\Omega \tilde{n}_\alpha \left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta \tilde{n}_\alpha} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta \tilde{n}_\alpha}\right) dV \\ &- \int_\Omega \left(\frac{\delta F}{\partial \omega_\alpha}\frac{\delta G}{\delta \tilde{n}_\alpha} - \frac{\delta G}{\delta \omega_\alpha}\frac{\delta F}{\delta \tilde{n}_\alpha}\right) dV \\ &- \int_\Omega \omega_\alpha \left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta \omega_\alpha} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta \omega_\alpha}\right) dV. \end{aligned} \tag{3.6}$$

The first, second and fourth terms in the above expression represent the effects of the material derivative on u, n and ω, respectively. The third term interrelates n and ω (anticipating that $\omega = \sigma\dot{n}$). The above expression is a Poisson bracket in that it satisfies the antisymmetry property and the Jacobi identity.

In order to find the appropriate Poisson bracket for the system where the vector $\tilde{n}$ is constrained to be a unit vector, we need to construct a projection mapping:

$$\tilde{n} \xrightarrow{P} \frac{\tilde{n}}{(\tilde{n}_\beta \tilde{n}_\beta)^{1/2}} \equiv n, \tag{3.7}$$

where we restrict ourselves to the functionals F and G which depend on $\tilde{n}$ only through their dependence on n. Thus we have

$$\frac{\delta F}{\delta \tilde{n}_\alpha} = \frac{\delta F}{\delta n_\beta}\frac{\partial n_\beta}{\partial \tilde{n}_\alpha} = \frac{1}{(\tilde{n}_\gamma \tilde{n}_\gamma)^{1/2}}(\delta_{\alpha\beta} - n_\beta n_\alpha)\frac{\delta F}{\delta n_\beta}. \tag{3.8}$$

Substitution of this expression into the Poisson bracket (3.6) yields

$$\{F, G\} = - \int_\Omega u_\alpha \left(\frac{\delta F}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta u_\alpha} - \frac{\delta G}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta u_\alpha} \right) dV$$

$$- \int_\Omega n_\alpha \left(\frac{\delta F}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta n_\alpha} - \frac{\delta G}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta n_\alpha} \right) dV$$

$$+ \int_\Omega n_\alpha \left(\frac{\delta F}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \left(n_\beta n_\alpha \frac{\delta G}{\delta n_\beta} \right) - \frac{\delta G}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \left(n_\beta n_\alpha \frac{\delta F}{\delta n_\beta} \right) \right) dV$$

$$- \int_\Omega \frac{1}{(\tilde{n}_\gamma \tilde{n}_\gamma)^{1/2}} \left(\frac{\delta F}{\delta \omega_\alpha} \frac{\delta G}{\delta n_\alpha} - \frac{\delta G}{\delta \omega_\alpha} \frac{\delta F}{\delta n_\alpha} \right) dV$$

$$+ \int_\Omega \frac{1}{(\tilde{n}_\gamma \tilde{n}_\gamma)^{1/2}} \left(\frac{\delta F}{\delta \omega_\alpha} n_\beta n_\alpha \frac{\delta G}{\delta n_\beta} - \frac{\delta G}{\delta \omega_\alpha} n_\beta n_\alpha \frac{\delta F}{\delta n_\beta} \right) dV$$

$$- \int_\Omega \omega_\alpha \left(\frac{\delta F}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta \omega_\alpha} - \frac{\delta G}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta \omega_\alpha} \right) dV, \tag{3.9}$$

which, by construction, must satisfy the properties of a Poisson bracket.

The functional derivatives in these expressions are defined as follows. The functional derivative of F with respect to the velocity is given by

$$\frac{\delta F}{\delta u_\alpha} \equiv \prod\nolimits_\alpha \left(\frac{\partial f}{\partial u_\alpha} \right), \tag{3.10}$$

where $\Pi(a)$ is the projection operator to the divergence-free space defined in Reference 12 as

$$\Pi(a) \equiv a - \nabla p \tag{3.11}$$

Note that $u = 0$ on the boundary of Ω, $\partial\Omega$, which implies (i.e., to allow a proper inner product[12]) that $\delta F/\delta u = 0$ on $\partial\Omega$ as well. The functional derivative of F with respect to the director is defined as

$$\frac{\delta F}{\delta n_\alpha} \equiv \frac{\partial f}{\partial n_\alpha} - \frac{\partial f}{\partial n_\beta} n_\beta n_\alpha - \left(\frac{\partial f}{\partial n_{\alpha,\beta}} \right)_{,\beta} + n_\alpha n_\gamma \left(\frac{\partial f}{\partial n_{\gamma,\beta}} \right)_{,\beta}, \tag{3.12}$$

since it must belong to the space where n is a unit vector. (Note that this definition implies that $n \cdot [\delta F/\delta n] = 0$). Finally, the remaining functional derivative is defined as simply

$$\frac{\delta F}{\delta \omega_\alpha} = \frac{\partial f}{\partial \omega_\alpha}. \tag{3.13}$$

From the definition of the derivative (3.12), it is now obvious that the bracket (3.9) reduces to Equation (3.6) when we set $n = \tilde{n}$. Thus the Poisson bracket is the same regardless of whether we consider n or $\tilde{n}$, provided that we use the proper functional derivative, (3.12).

The dissipation bracket, $[\cdot\,,\cdot]$, in Equation (3.5) is expressed as

$$[F, G] \equiv \int_\Omega Q_{\alpha\beta\gamma\varepsilon} \frac{\partial}{\partial r_\alpha}\left(\frac{\delta F}{\delta u_\beta}\right) \frac{\partial}{\partial r_\gamma}\left(\frac{\delta G}{\delta u_\varepsilon}\right) dV$$
$$- \int_\Omega \alpha_2 \left[\frac{\delta F}{\delta \omega_\alpha} - \frac{\partial}{\partial r_\beta}\left(\frac{\delta F}{\delta u_\alpha}\right) n_\beta\right]\left[\frac{\delta G}{\delta \omega_\alpha} - \frac{\partial}{\partial r_\gamma}\left(\frac{\delta G}{\delta u_\alpha}\right) n_\gamma\right] dV$$
$$+ \int_\Omega \alpha_3 \left[\frac{\delta F}{\delta \omega_\alpha} + \frac{\partial}{\partial r_\alpha}\left(\frac{\delta F}{\delta u_\beta}\right) n_\beta\right]\left[\frac{\delta G}{\delta \omega_\alpha} + \frac{\partial}{\partial r_\alpha}\left(\frac{\delta G}{\delta u_\gamma}\right) n_\gamma\right] dV, \quad (3.14)$$

where the phenomenological matrix, $\mathbf{Q}$, is given by

$$Q_{\alpha\beta\gamma\varepsilon} = \alpha_1 n_\alpha n_\beta n_\gamma n_\varepsilon + \alpha_4(\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\beta\gamma}\delta_{\alpha\varepsilon})/2$$
$$+ (\alpha_2 + \alpha_5)(\delta_{\beta\varepsilon} n_\alpha n_\gamma + \delta_{\beta\gamma} n_\alpha n_\varepsilon)/2$$
$$+ (\alpha_6 - \alpha_3)(\delta_{\alpha\varepsilon} n_\beta n_\gamma + \delta_{\alpha\gamma} n_\beta n_\varepsilon)/2. \quad (3.15)$$

This matrix is the most general possible form, out to fourth order in n, for an incompressible fluid. The first term in the dissipation bracket, (3.14), represents translational dissipation effects, and has the form of the dissipation of the transversely isotropic fluid.[1] The second and third terms represent the dissipation effects of rotational motion, i.e., they possess the forms of the upper- and lower-convected derivatives, respectively. Note that this bracket couples the variables ω and u with themselves, and each other. n does not appear in the dissipation bracket since it is a conserved quantity when the time scale of the problem is such that the inertial effects are present. Due to the nature of $\ddot{n}$, $\dot{n}$ must satisfy Equation (2.4) and the dissipation shows itself in the equation for angular momentum.

The above dissipation bracket provides for the Hamiltonian, defined by Equation (3.3), the same dissipation (provided that ω is set equal to $\dot{n}$) as that which was evaluated by Leslie[5] (Clausius-Duhem inequality):

$$dH/dt = -[H, H] = -\int_\Omega t_{\alpha\beta} A_{\alpha\beta}\, dV + \int_\Omega g_\alpha N_\alpha\, dV \leq 0, \quad (3.16)$$

where $t_{\alpha\beta}$ and g are defined by Equations (2.9) and (2.15), respectively, since the Parodi relationship holds. (In fact, it can immediately be seen now that this relation is implied from Equation (3.15): since $\mathbf{Q}$ is a phenomenological dissipative parameter, it must satisfy the fundamental theorem of Onsager as well as material invariance; $Q_{\alpha\beta\gamma\varepsilon} = Q_{\gamma\varepsilon\alpha\beta} = Q_{\beta\alpha\gamma\varepsilon} = Q_{\alpha\beta\varepsilon\gamma}$.) As a consequence, the non-negative-definite nature of the dissipation bracket imposes the same restrictions on the parameters α_i as appear in the LE theory (Equation 35 of Reference 5). (See Appendix C for a note on this calculation). Also note that the dissipation is expressed by Equations (3.14–16) solely in terms of objective quantities.

Using the formalism developed in References 11, 12 and the references therein, we can write the functional derivatives of the Hamiltonian (3.3) as

$$\frac{\delta H}{\delta u_\alpha} = u_\alpha, \tag{3.17a}$$

$$\frac{\delta H}{\delta n_\alpha} = -\chi_a n_\beta H_\beta H_\alpha + \chi_a n_\beta n_\gamma H_\beta H_\gamma n_\alpha + \frac{\partial W}{\partial n_\alpha} - \left(\frac{\partial W}{\partial n_{\alpha,\gamma}}\right)_{,\gamma} - \frac{\partial W}{\partial n_\beta} n_\beta n_\alpha + \left(\frac{\partial W}{\partial n_{\beta,\gamma}}\right)_{,\gamma} n_\beta n_\alpha, \tag{3.17b}$$

and

$$\frac{\delta H}{\delta \omega_\alpha} = \frac{1}{\sigma}\,\omega_\alpha, \tag{3.17c}$$

so that the following evolution equations can be derived from Equations, (3.2, 3, 5, 6, 14):

$$\dot{u}_\alpha = F_\alpha - p_{,\alpha} - \left(\frac{\partial W}{\partial n_{\beta,\gamma}}\, n_{\beta,\alpha}\right)_{,\gamma} + t'_{\alpha\gamma,\gamma}, \tag{3.18}$$

$$\frac{\partial n_\alpha}{\partial t} = -u_\gamma n_{\alpha,\gamma} + \frac{1}{\sigma}(\omega_\alpha - \omega_\beta n_\beta n_\alpha), \tag{3.19}$$

$$\frac{\partial \omega_\alpha}{\partial t} = -u_\gamma \omega_{\alpha,\gamma} - \frac{\partial W}{\partial n_\alpha} + \frac{\partial W}{\partial n_\beta} n_\beta n_\alpha + \left(\frac{\partial W}{\partial n_{\alpha,\beta}}\right)_{,\beta} - \left(\frac{\partial W}{\partial n_{\gamma,\beta}}\right)_{,\beta} n_\gamma n_\alpha + G_\alpha - G_\beta n_\beta n_\alpha + \alpha_2\left[\frac{1}{\sigma}\,\omega_\alpha - u_{\alpha,\gamma} n_\gamma\right] - \alpha_3\left[\frac{1}{\sigma}\,\omega_\alpha + u_{\gamma,\alpha} n_\gamma\right], \tag{3.20}$$

where $t'_{\alpha\gamma}$ is defined by Equation (2.9) with ω/σ replacing $\dot{n}$. From Equation (3.19), we get

$$\sigma \dot{n}_\alpha = \omega_\alpha - \omega_\beta n_\beta n_\alpha \rightarrow \omega_\alpha = \sigma \dot{n}_\alpha + \varepsilon n_\alpha, \tag{3.21}$$

with the parameter $\varepsilon = \omega_\beta n_\beta$, as yet, not specified. In order to get $\sigma \ddot{n}_\alpha$, we take the material derivative of Equation (3.21):

$$\sigma \ddot{n}_\alpha = \dot{\omega}_\alpha - \dot{\omega}_\beta n_\beta n_\alpha - \omega_\beta \dot{n}_\beta n_\alpha - \varepsilon \dot{n}_\alpha. \tag{3.22}$$

Substitution of Equation (3.20) into the above expression then yields

$$\sigma \ddot{n}_\alpha = G_\alpha + \gamma n_\alpha - \frac{\partial W}{\partial n_\alpha} + \left(\frac{\partial W}{\partial n_{\alpha,\beta}}\right)_{,\beta} + g_\alpha - \varepsilon \dot{n}_\alpha, \tag{3.23}$$

where the parameter γ is evaluated as Equation (2.16). From the definition of the Hamiltonian provided by Equation (3.3), we can now specify the parameter $\varepsilon = \sigma \dot{n}_\beta n_\beta = 0$ from the initial condition $\omega = \sigma \dot{n}$ and Equation (3.21). For this value of ε, Equations (3.18, 23) reduce exactly to the LE equations, Equations (2.2, 3).

3.2 Non-Inertial Theory

It is also possible to use the generalized bracket formalism in order to develop the LE equations under the quasi-steady state approximation—Equations (2.2, 19, 20). For this purpose, the Poisson bracket and dissipation expressions, developed in the last subsection, need to be modified accordingly.

We shall now assume that the time scale of the problem is such that the director inertia is negligible, i.e., $\sigma \to 0 \Rightarrow \omega = 0$. As such, the number of primary variables in our problem is reduced from three to two:

$$F[u, n] = \int_\Omega f(u, n)\, dV, \tag{3.24}$$

and consequently, the Hamiltonian becomes

$$H[u, n] = \int_\Omega \left(\frac{1}{2} u \cdot u + W + \psi_m\right) dV. \tag{3.25}$$

From Equation (3.6), we know that the inertial Poisson bracket is given as

$$\begin{aligned}
\{F, G\} = &- \int_\Omega u_\alpha \left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta u_\alpha} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta u_\alpha}\right) dV \\
&- \int_\Omega n_\alpha \left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta n_\alpha} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta n_\alpha}\right) dV \\
&- \int_\Omega \left(\frac{\delta F}{\delta(\sigma \dot{n}_\alpha)}\frac{\delta G}{\delta n_\alpha} - \frac{\delta G}{\delta(\sigma \dot{n}_\alpha)}\frac{\delta F}{\delta n_\alpha}\right) dV \\
&- \int_\Omega \sigma \dot{n}_\alpha \left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta(\sigma \dot{n}_\alpha)} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta(\sigma \dot{n}_\alpha)}\right) dV,
\end{aligned} \tag{3.26}$$

where we have replaced ω_α with $\sigma \dot{n}_\alpha$. As $\sigma \to 0$, the fourth integral in this expression vanishes, however, we still have the functional derivatives with respect to $\sigma \dot{n}$ in the third integral which must be reduced in terms of u and n. In order to accomplish this task, let us invoke the conservative equation of continuity for the vector n:

$$\dot{n}_\alpha = n_\gamma u_{\alpha,\gamma}, \tag{3.27}$$

where we have used the upper-convected derivative for a vectorial quantity to take into account the codeformation with the medium. Next, we set

$$\frac{\delta H}{\delta(\dot{n}_\alpha)} = \dot{n}_\alpha = n_\gamma \frac{\partial}{\partial r_\gamma} \frac{\delta H}{\delta u_\alpha}, \tag{3.28}$$

for any H which depends on u only through the kinetic energy, as is the case for the Hamiltonian (3.25). Substituting this expression, written for functionals $F = H$ and $G = H$ into the bracket, (3.26), yields the Poisson bracket for the functionals $F[u, n]$ and $G[u, n]$:

$$\begin{aligned} \{F, G\} = &- \int_\Omega u_\alpha \left(\frac{\delta F}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta u_\alpha} - \frac{\delta G}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta u_\alpha} \right) dV \\ &- \int_\Omega n_\alpha \left(\frac{\delta F}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta n_\alpha} - \frac{\delta G}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta n_\alpha} \right) dV \\ &- \int_\Omega n_\gamma \left(\frac{\delta G}{\delta n_\alpha} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta u_\alpha} - \frac{\delta F}{\delta n_\alpha} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta u_\alpha} \right) dV. \end{aligned} \tag{3.29}$$

Thus we arrive at the materially-objective Poisson bracket for a liquid-crystalline system in terms of functionals of the primary variables u and n. Note that this bracket applies whether or not n is constrained to be a unit vector. Similarly to §3.1, it is easy to show that applying the map (3.7) to the unconstrained bracket yields an additional term, which vanishes under the definition (3.12).

In order to develop the proper dissipation bracket, we must consider the changes which occur in the problem as we adjust the time scale to allow the neglect of the system inertia. The concept of a time scale is very important in determining which variables couple in the dissipation bracket. For example, if the time scale is particularly short, any phenomena occurring over a longer time scale are "fixed" in the system, and may be ignored. Alternatively, any phenomena occurring on a much shorter time scale will happen so rapidly as to reveal an "average" value, which also appears fixed. Thus, as we adjust our time scale to a value where the inertia can safely be neglected, the dissipation manifests itself in a different way. In terms of the dissipation bracket, the variables u and n now couple with themselves and each other, similarly to the previous case:

$$\begin{aligned} [F, G] = &\int_\Omega Q^n_{\alpha\beta\gamma\varepsilon} \frac{\partial}{\partial r_\alpha} \left(\frac{\delta F}{\delta u_\beta} \right) \frac{\partial}{\partial r_\gamma} \left(\frac{\delta G}{\delta u_\varepsilon} \right) dV + \int_\Omega P_{\alpha\beta\gamma\varepsilon} \frac{\delta F}{\delta n_\alpha} n_\beta \frac{\delta G}{\delta n_\gamma} n_\varepsilon \, dV \\ &+ \int_\Omega L_{\alpha\beta\gamma\varepsilon} \left(\frac{\partial}{\partial r_\alpha} \left(\frac{\delta F}{\partial u_\beta} \right) n_\gamma \frac{\delta G}{\delta n_\varepsilon} - \frac{\partial}{\partial r_\alpha} \left(\frac{\delta G}{\delta u_\beta} \right) n_\gamma \frac{\delta F}{\delta n_\varepsilon} \right) dV, \end{aligned} \tag{3.30}$$

where

$$Q^n_{\alpha\beta\gamma\varepsilon} = \beta^n_1 n_\alpha n_\beta n_\gamma n_\varepsilon + \beta^n_2(\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\beta\gamma}\delta_{\alpha\varepsilon})/2$$
$$+ \beta^n_3(\delta_{\alpha\varepsilon}n_\beta n_\gamma + \delta_{\beta\varepsilon}n_\alpha n_\gamma + \delta_{\alpha\gamma}n_\beta n_\varepsilon + \delta_{\beta\gamma}n_\alpha n_\varepsilon)/2, \quad (3.31)$$

$$P_{\alpha\beta\gamma\varepsilon} = \frac{1}{(\alpha_3 - \alpha_2)}[\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\beta\gamma}\delta_{\alpha\varepsilon}], \quad (3.32)$$

and

$$L_{\alpha\beta\gamma\varepsilon} = \frac{\alpha_3}{(\alpha_2 - \alpha_3)}[\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\alpha\varepsilon}\delta_{\beta\gamma}]. \quad (3.33)$$

Previously, no dissipation was allowed in the $\dot{n}$ equation, however, as we alter the time scale to neglect inertia, the dissipation must appear here. Thus the second term in the dissipation bracket represents relaxational phenomena, while the third allows for any non-affine coupling between the director and the velocity gradient. (See Appendix B for a discussion concerning the minus sign in the third term of the dissipation bracket). This dissipation bracket has exactly the same form as the previous bracket, (3.14), although at first glance this does not appear to be the case. The above form is a simpler representation of the standard form, which we wrote out at length in Equation (3.14) in order to illustrate the rotational nature of the previous dissipation. Here, however, we revert to the more elegant expression of Equation (3.30). Of course, the phenomenological coefficients are not the same as in the previous bracket, but this is to be expected. The dissipation terms represent the effect of the lumped (non-resolved) degrees of freedom in the overall energy balance. As such, they change as the accounted degrees of freedom change.

Through the identity $[H, H] \geq 0$, and the procedure of Appendix C, we can arrive at the following conditions on the phenomenological coefficients:

$$\alpha_3 - \alpha_2 \geq 0, \quad (3.34a)$$

$$\beta^n_2 \geq 0, \quad (3.34b)$$

$$\beta^n_3 + \beta^n_2 \geq 0, \quad (3.34c)$$

and

$$2(\beta^n_1 + 2\beta^n_3) + 3\beta^n_2 \geq 0. \quad (3.34d)$$

Upon substitution of Equation (2.22) into these inequalities, they become the equivalent inequalities of Leslie.[5]

Using the Poisson bracket, (3.29), and the above dissipation bracket, (3.30), the dynamical equation, (3.2), can be shown to be equivalent to the non-inertial LE equations (2.2, 19, 20). Thus we have arrived at a generalized bracket formalism for each particular case of the LE theory, and in so doing, we have realized the underlying structure and symmetry common to each case.

4. GENERALIZED BRACKET FORMULATION IN TERMS OF TENSORIAL PARAMETERS

Now that we recognize the inherent, underlying structure of the brackets for liquid-crystalline systems, we may reformulate these brackets in terms of tensorial parameters which better reflect the symmetries of liquid crystals. For instance, a turn of the director by 180 degrees (i.e., a change in sign of the director) does not influence the state of the material. The only way by which this insensitivity of the material to changes in sign of the director can be reflected into the equations is if we require them to depend on the tensor structural parameter, $\mathbf{m}$,

$$\mathbf{m} \equiv nn, \tag{4.1}$$

and its time derivative(s). However, the above equation for $\mathbf{m}$ is overly restrictive assuming a perfect alignment of the molecules along the director axis n.

In general, a distribution of different orientations is established, in which case Equation (4.1) should be replaced by an average of nn over the distribution function. In this case, only the more general constraint

$$tr(\mathbf{m}) = 1, \tag{4.2}$$

is applicable. In addition to allowing the correct representation of the molecular symmetries into the equations, a reformulation in terms of a general, symmetric tensor parameter, $\mathbf{m}$, subject to the constraint (4.2), allows the description of a wider variety of liquid-crystalline structures: nematic, cholesteric and blue phases,[6] as well as states with limited (statistical) order as encountered in polymeric liquid crystals.[6] In addition, this formulation allows the description of various liquid-crystalline states at equilibrium and the transitions among these states[6,9,14]. This is only feasible through a unique description of the material's free energy in terms of the various moments of $\mathbf{m}$ and its spatial gradients. Note that this is not possible if Equation (4.1) is valid (or, which is equivalent, if we still consider the problem in terms of a unit vector description of the material), since in that case all the moments are equal to unity. Indeed, this has been performed before[13,14] by incorporating a Landau-de Gennes expansion of the bulk free energy into the Hamiltonian of the form

$$H_b \equiv \int_\Omega (a_2 m_{\alpha\beta} m_{\beta\alpha} + a_3 m_{\alpha\beta} m_{\beta\gamma} m_{\gamma\alpha} + a_4 m_{\alpha\beta} m_{\beta\gamma} m_{\gamma\varepsilon} m_{\varepsilon\alpha}) \, dV, \tag{4.3}$$

where the a_i are phenomenological coefficients which depend on the system temperature and concentration. (Due to the Cayley-Hamilton theorem, only terms out to fourth order are independent). This expression has been used many times in the past to describe phase transitions in liquid-crystalline systems[6,9,10,13,14,23,24] for static problems, however, no such expression is possible in terms of n since the unit vector constraint will always reduce an equivalent Equation (4.3) to a constant. In this section, we shall neglect H_b and consider only an equivalent free energy (Hamiltonian) to Equations (3.3, 25). We shall return to discuss the significance of H_b in §5, however.

When $\mathbf{m}$ can be represented as nn, it corresponds to a uniaxial structure, however, a more general representation requires two independent directions $vv + nn$ corresponding to a biaxial structure. Furthermore, it is well known that even in the nematic liquid-crystalline state the uniaxial state is unstable relative to the biaxial one,[6] although the second component is much smaller in magnitude and can usually be neglected.

Based upon the results of §3, we shall now attempt to derive generalized equations for liquid crystals in terms of the tensor $\mathbf{m}$. The procedure is completely analogous to that of §3, and therefore the discussion will be kept to a minimum.

4.1 Inertial Theory

Now we shall consider a liquid crystalline material which is described by the velocity vector, u, and two tensor fields, $\mathbf{m}$ and $\mathbf{w}$. As before, we shall later set $w_{\alpha\beta} = \sigma^m \dot{m}_{\alpha\beta}$, the material derivative of the structure tensor, $m_{\alpha\beta}$, multiplied by a different inertial constant, σ^m. We can therefore write an arbitrary functional of these three variable fields as

$$F[u, \mathbf{m}, \mathbf{w}] \equiv \int_\Omega f(u, \mathbf{m}, \mathbf{w})\, dV. \tag{4.4}$$

Once again, we can write the dynamical equation for this functional as

$$\frac{dF}{dt} = \{(F, H)\} \equiv \{F, H\} - [F, H], \tag{4.5}$$

where the Hamiltonian is given by

$$H[u, \mathbf{m}, \mathbf{w}] \equiv \int_\Omega \left(\frac{1}{2} \rho u \cdot u + \frac{1}{2\sigma^m} \mathbf{w} : \mathbf{w} + W + \psi_m \right) dV. \tag{4.6}$$

In this Hamiltonian, ρ is again taken to be unity using suitable units for mass and length, in order to simplify the final expressions. Similarly, ψ_m and W (see Reference 25 for details) are now expressed in terms of $\mathbf{m}$ (neglecting higher-order terms):

$$\psi_m \equiv -\frac{1}{2} [\chi_a HH : \mathbf{m} + \chi_\perp H \cdot H], \tag{4.7}$$

and

$$W \equiv \frac{1}{2} b_1 m_{\alpha\beta,\gamma} m_{\alpha\beta,\gamma} + \frac{1}{2} b_2 m_{\alpha\beta,\alpha} m_{\gamma\beta,\gamma}. \tag{4.8}$$

We can now write the inertial Poisson bracket for two arbitrary functionals $F[u_\alpha, \tilde{m}_{\alpha\beta}, w_{\alpha\beta}]$ and $G[u_\alpha, \tilde{m}_{\alpha\beta}, w_{\alpha\beta}]$, where $\tilde{m}_{\alpha\beta}$ is the unconstrained version of $m_{\alpha\beta}$, as

$$\begin{aligned}\{F, G\} = &- \int_\Omega u_\alpha \left(\frac{\delta F}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta u_\alpha} - \frac{\delta G}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta u_\alpha}\right) dV \\ &- \int_\Omega \tilde{m}_{\alpha\beta} \left(\frac{\delta F}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta \tilde{m}_{\alpha\beta}} - \frac{\delta G}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta \tilde{m}_{\alpha\beta}}\right) dV \\ &- \int_\Omega \left(\frac{\delta F}{\delta w_{\alpha\beta}} \frac{\delta G}{\delta \tilde{m}_{\alpha\beta}} - \frac{\delta G}{\delta w_{\alpha\beta}} \frac{\delta F}{\delta \tilde{m}_{\alpha\beta}}\right) dV \\ &- \int_\Omega w_{\alpha\beta} \left(\frac{\delta F}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta w_{\alpha\beta}} - \frac{\delta G}{\delta u_\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta w_{\alpha\beta}}\right) dV.\end{aligned} \tag{4.9}$$

It can be shown that the above expression satisfies both the antisymmetry property and the Jacobi identity for a Poisson bracket.

In order to obtain the appropriate Poisson bracket that satisfies both of the above properties under the constraint imposed by Equation (4.2), we need to modify the bracket (4.9). For this purpose, we once again introduce a mapping:

$$\tilde{m}_{\alpha\beta} \xrightarrow{P_m} \frac{\tilde{m}_{\alpha\beta}}{\tilde{m}_{\gamma\gamma}} \equiv m_{\alpha\beta}, \tag{4.10}$$

which projects an arbitrary tensor to a tensor with unit trace. We note that for any functional, F, which depends on $\tilde{m}_{\alpha\beta}$ only through $m_{\alpha\beta}$,[13]

$$\frac{\delta F}{\delta \tilde{m}_{\alpha\beta}} = \frac{\delta F}{\delta m_{\gamma\varepsilon}} \frac{\partial m_{\gamma\varepsilon}}{\partial \tilde{m}_{\alpha\beta}} = \frac{\delta F}{\delta m_{\gamma\varepsilon}} \frac{1}{\tilde{m}_{\gamma\gamma}} (\delta_{\alpha\gamma}\delta_{\beta\varepsilon} - m_{\gamma\varepsilon}\delta_{\alpha\beta}). \tag{4.11}$$

Substitution of the mapping (4.11) into the bracket (4.9) yields the Poisson bracket for the constrained tensor, $\mathbf{m}$[13]:

$$\{F, G\} = -\int_\Omega u_\alpha \left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta u_\alpha} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta u_\alpha}\right) dV$$

$$-\int_\Omega m_{\alpha\beta}\left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta m_{\alpha\beta}} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta m_{\alpha\beta}}\right) dV$$

$$-\int_\Omega \left(\frac{\delta F}{\delta w_{\alpha\beta}}\frac{\delta G}{\delta m_{\alpha\beta}} - \frac{\delta G}{\delta w_{\alpha\beta}}\frac{\delta F}{\delta m_{\alpha\beta}}\right) dV$$

$$+\int_\Omega m_{\gamma\varepsilon}\left(\frac{\delta F}{\delta w_{\alpha\alpha}}\frac{\delta G}{\delta m_{\gamma\varepsilon}} - \frac{\delta G}{\delta w_{\alpha\alpha}}\frac{\delta F}{\delta m_{\gamma\varepsilon}}\right) dV$$

$$-\int_\Omega w_{\alpha\beta}\left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta w_{\alpha\beta}} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta w_{\alpha\beta}}\right) dV, \tag{4.12}$$

where F and G are now functionals of u, $\mathbf{m}$ and $\mathbf{w}$. In the above expression, the functional derivatives are defined as follows:

$$\frac{\delta F}{\delta u_\alpha} \equiv \prod\nolimits_\alpha \left(\frac{\partial f}{\partial u_\alpha}\right), \tag{4.13}$$

$$\frac{\delta F}{\delta m_{\alpha\beta}} \equiv \frac{1}{2}\left(\frac{\partial f}{\partial m_{\alpha\beta}} + \frac{\partial f}{\partial m_{\beta\alpha}}\right) - \frac{1}{3}\delta_{\alpha\beta}\frac{\partial f}{\partial m_{\gamma\gamma}},$$
$$-\frac{1}{2}\left(\frac{\partial f}{\partial m_{\alpha\beta,\gamma}}\right)_{,\gamma} - \frac{1}{2}\left(\frac{\partial f}{\partial m_{\beta\alpha,\gamma}}\right)_{,\gamma} + \frac{1}{3}\delta_{\alpha\beta}\left(\frac{\partial f}{\partial m_{\varepsilon\varepsilon,\gamma}}\right)_{,\gamma}, \tag{4.14}$$

and

$$\frac{\delta F}{\delta w_{\alpha\beta}} \equiv \frac{\partial f}{\partial w_{\alpha\beta}}. \tag{4.15}$$

Note that no constraint is imposed *a priori* on the tensor parameter $\mathbf{w}$.

A dissipation bracket can also be provided, analogously to the bracket (3.14), as

$$[F, G] \equiv \int_\Omega R_{\alpha\beta\gamma\varepsilon} \frac{\partial}{\partial r_\alpha}\left(\frac{\delta F}{\delta u_\beta}\right) \frac{\partial}{\partial r_\gamma}\left(\frac{\delta G}{\delta u_\varepsilon}\right) dV$$

$$- \int_\Omega \alpha_2^m \left[\frac{\delta F}{\delta w_{\alpha\beta}} - m_{\alpha\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta u_\beta} - m_{\beta\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta F}{\delta u_\alpha}\right]$$

$$\cdot \left[\frac{\delta G}{\delta w_{\alpha\beta}} - m_{\alpha\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta u_\beta} - m_{\beta\gamma} \frac{\partial}{\partial r_\gamma} \frac{\delta G}{\delta u_\alpha}\right] dV$$

$$+ \int_\Omega \alpha_3^m \left[\frac{\delta F}{\delta w_{\alpha\beta}} + m_{\alpha\gamma} \frac{\partial}{\partial r_\beta} \frac{\delta F}{\delta u_\gamma} + m_{\beta\gamma} \frac{\partial}{\partial r_\alpha} \frac{\delta F}{\delta u_\gamma}\right]$$

$$\cdot \left[\frac{\delta G}{\delta w_{\alpha\beta}} + m_{\alpha\gamma} \frac{\partial}{\partial r_\beta} \frac{\delta G}{\delta u_\gamma} + m_{\beta\gamma} \frac{\partial}{\partial r_\alpha} \frac{\delta G}{\delta u_\gamma}\right] dV, \tag{4.16}$$

where

$$R_{\alpha\beta\gamma\varepsilon} \equiv \alpha_1^m(m_{\alpha\gamma}m_{\beta\varepsilon} + m_{\alpha\varepsilon}m_{\beta\gamma})/2 + \alpha_4^m(\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\beta\gamma}\delta_{\alpha\varepsilon})/2$$
$$+ \alpha_5^m(\delta_{\beta\varepsilon}m_{\alpha\gamma} + \delta_{\beta\gamma}m_{\alpha\varepsilon} + \delta_{\alpha\varepsilon}m_{\beta\gamma} + \delta_{\alpha\gamma}m_{\beta\varepsilon})/2$$
$$+ \alpha_6^m(m_{\alpha\zeta}m_{\zeta\gamma}\delta_{\beta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}\delta_{\beta\gamma} + \delta_{\alpha\gamma}m_{\beta\zeta}m_{\zeta\varepsilon} + \delta_{\alpha\varepsilon}m_{\beta\zeta}m_{\zeta\gamma})/2$$
$$+ \alpha_7^m(m_{\alpha\zeta}m_{\zeta\gamma}m_{\beta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}m_{\beta\gamma} + m_{\alpha\gamma}m_{\beta\zeta}m_{\zeta\varepsilon} + m_{\alpha\varepsilon}m_{\beta\zeta}m_{\zeta\gamma})/2$$
$$+ \alpha_8^m(m_{\alpha\zeta}m_{\zeta\gamma}m_{\beta\eta}m_{\eta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}m_{\beta\eta}m_{\eta\gamma})/2. \tag{4.17}$$

Note that the above expression is the most general form of the phenomenological tensor **R** (for an incompressible fluid), given the unit trace constraint on **m** and the Cayley-Hamilton theorem. (The eight coefficients α_i^m can, in general, be functions of the second and third invariants of **m**).

Using Equations (4.6–8, 13–15), we may evaluate the functional derivatives of the Hamiltonian:

$$\frac{\delta H}{\delta u_\alpha} = u_\alpha, \tag{4.18a}$$

$$\frac{\delta H}{\delta m_{\alpha\beta}} = -\frac{1}{2}\chi_a\left(H_\alpha H_\beta - \frac{1}{3}\delta_{\alpha\beta}H_\gamma H_\gamma\right) - b_1 m_{\alpha\beta,\gamma,\gamma}$$
$$- b_2\left(\frac{1}{2}m_{\beta\gamma,\alpha} + \frac{1}{2}m_{\alpha\gamma,\beta} - \frac{1}{3}\delta_{\alpha\beta}m_{\gamma\varepsilon,\varepsilon}\right)_{,\gamma}, \tag{4.18b}$$

and

$$\frac{\delta H}{\delta w_{\alpha\beta}} = w_{\alpha\beta}/\sigma^m. \tag{4.18c}$$

Upon substitution of the above derivatives into the dynamical equation provided by Equations (4.5, 12, 16), we obtain the evolution equations

$$\dot{u}_\alpha = F^m_\alpha - p,_\alpha - \left(m_{\gamma\varepsilon,\alpha}\frac{\partial W}{\partial m_{\gamma\varepsilon,\beta}}\right)_{,\beta} + T_{\alpha\beta,\beta}, \tag{4.19}$$

$$\sigma^m \dot{m}_{\alpha\beta} = w_{\alpha\beta} - w_{\gamma\gamma}m_{\alpha\beta} \rightarrow w_{\alpha\beta} = \sigma^m\dot{m}_{\alpha\beta} + \varepsilon m_{\alpha\beta}, \tag{4.20}$$

$$\dot{w}_{\alpha\beta} = -\frac{\delta H}{\delta m_{\alpha\beta}} + \delta_{\alpha\beta}m_{\gamma\varepsilon}\frac{\delta H}{\delta m_{\gamma\varepsilon}} + \alpha^m_2\left[\frac{1}{\sigma^m}w_{\alpha\beta} - m_{\alpha\gamma}u_{\beta,\gamma} - m_{\beta\gamma}u_{\alpha,\gamma}\right]$$
$$- \alpha^m_3\left[\frac{1}{\sigma^m}w_{\alpha\beta} + m_{\alpha\gamma}u_{\gamma,\beta} + m_{\beta\gamma}u_{\gamma,\alpha}\right], \tag{4.21}$$

where

$$F^m_\alpha = \chi_a H_\beta H_{\gamma,\alpha}m_{\beta\gamma}, \tag{4.22}$$

and

$$T_{\alpha\beta} = R_{\beta\alpha\gamma\varepsilon}A_{\gamma\varepsilon} + 2\alpha^m_2 m_{\beta\gamma}\left[\frac{1}{\sigma^m}w_{\alpha\gamma} - m_{\alpha\varepsilon}u_{\gamma,\varepsilon} - m_{\varepsilon\gamma}u_{\alpha,\varepsilon}\right]$$
$$+ 2\alpha^m_3 m_{\alpha\gamma}\left[\frac{1}{\sigma^m}w_{\beta\gamma} + m_{\gamma\varepsilon}u_{\varepsilon,\beta} + m_{\beta\varepsilon}u_{\varepsilon,\gamma}\right]. \tag{4.23}$$

From Equations (4.20, 21), we obtain

$$\sigma^m\ddot{m}_{\alpha\beta} = \dot{w}_{\alpha\beta} - \dot{w}_{\gamma\gamma}m_{\alpha\beta} - w_{\gamma\gamma}\dot{m}_{\alpha\beta} = -\frac{\delta H}{\delta m_{\alpha\beta}} - 3m_{\gamma\varepsilon}\frac{\delta H}{\delta m_{\gamma\varepsilon}}\left(m_{\alpha\beta} - \frac{1}{3}\delta_{\alpha\beta}\right)$$
$$+ (\alpha^m_2 - \alpha^m_3)\dot{m}_{\alpha\beta} - \alpha^m_2[m_{\alpha\gamma}u_{\beta,\gamma} + m_{\beta\gamma}u_{\alpha,\gamma}]$$
$$- \alpha^m_3[m_{\alpha\gamma}u_{\gamma,\beta} + m_{\beta\gamma}u_{\gamma,\alpha}] + 2(\alpha^m_2 + \alpha^m_3)m_{\alpha\beta}m_{\gamma\varepsilon}u_{\gamma,\varepsilon} - \varepsilon\dot{m}_{\alpha\beta}. \tag{4.24}$$

Setting $\varepsilon = w_{\gamma\gamma} = \dot{m}_{\gamma\gamma} = 0$, we obtain the generalized theory in terms of tensorial parameters.

If we take the special case of Equation (4.1), i.e.,

$$m_{\alpha\beta} = n_\alpha n_\beta, \qquad \dot{m}_{\alpha\beta} = \dot{n}_\alpha n_\beta + n_\alpha \dot{n}_\beta \quad \text{and} \quad \ddot{m}_{\alpha\beta} = \ddot{n}_\alpha n_\beta + n_\alpha \ddot{n}_\beta + 2\dot{n}_\alpha \dot{n}_\beta, \tag{4.25}$$

then we can transform the above tensorial equations directly into the inertial LE equations in the following manner. First we must pick up the parameters as such[25]:

$$K_1 = K_3 = 2b_1 + b_2, \qquad K_2 = 2b_1, \qquad \sigma = 2\sigma^m,$$

$$\alpha_1 + \alpha_2 - \alpha_3 = \alpha_1^m + \alpha_8^m + 2\alpha_7^m, \qquad \alpha_2 + \alpha_5 = \alpha_5 - \alpha_3 = \alpha_6^m + \alpha_6^m,$$

$$\alpha_4 = \alpha_4^m, \qquad \alpha_2/2 = \alpha_2^m, \qquad \text{and} \qquad \alpha_3/2 = \alpha_3^m. \tag{4.26}$$

Note that the choice of σ provides the same rotational kinetic energy in the two Hamiltonian expressions when $\mathbf{m} = nn$, as can be seen explicitly by expanding the rotational kinetic energy of Equation (4.6) for $\mathbf{m} = nn$:

$$w_{\alpha\beta}w_{\alpha\beta}/2\sigma^m = \sigma^m(\dot{n}_\alpha n_\beta + n_\alpha \dot{n}_\beta)(\dot{n}_\alpha n_\beta + n_\alpha \dot{n}_\beta)/2 = \sigma^m \dot{n}_\alpha \dot{n}_\alpha = \omega_\alpha \omega_\alpha/4\sigma^m. \tag{4.27}$$

Therefore, in order for Equation (4.27) to be equivalent to the rotational kinetic energy of Equation (3.3), we must have $\sigma = 2\sigma^m$. Similarly, for a unit vector description, we know that

$$n_\alpha \ddot{n}_\alpha + \dot{n}_\alpha \dot{n}_\alpha = 0. \tag{4.28}$$

In terms of the tensor $\ddot{m}_{\alpha\beta}$, this becomes

$$n_\alpha n_\beta \ddot{m}_{\alpha\beta} = 2\ddot{n}_\alpha n_\alpha = -2\dot{n}_\alpha \dot{n}_\alpha, \tag{4.29}$$

but according to Equation (4.24), we have

$$\sigma^m n_\alpha n_\beta \ddot{m}_{\alpha\beta} = -3 n_\alpha n_\beta \frac{\delta H}{\delta m_{\alpha\beta}}. \tag{4.30}$$

Therefore, in order to make the transformation from $\mathbf{m}$ to n, we must realize that

$$-3 n_\alpha n_\beta \frac{\delta H}{\delta m_{\alpha\beta}} = -2\sigma^m \dot{n}_\alpha \dot{n}_\alpha. \tag{4.31}$$

This equality must hold for the $\mathbf{m} \to n$ transformation to be valid since the $\mathbf{m}$-level description contains additional information which must be constrained to allow the transition to the vector level. One more point—because of the difference in the constraints between the vector and tensor cases, we need to express the functional derivative $\delta H/\delta n$ in terms of the functional derivatives $\delta H/\delta \mathbf{m}$ through the relation

$$\frac{\delta H}{\delta n_\alpha} = 2\frac{\delta H}{\delta m_{\gamma\alpha}} n_\gamma - 2\frac{\delta H}{\delta m_{\beta\gamma}} n_\beta n_\gamma n_\alpha, \tag{4.32}$$

obtained by differentiation by parts of the partial derivatives and the use of the corresponding projection operations. Once the above points are taken into account, it is easy to show that the general tensor theory reduces exactly to the LE theory, Equations (2.2, 3), in the limit $\mathbf{m} = nn$.

4.2 Non-Inertial Theory

Now we may apply the procedure of §3.2 to the generalized tensorial theory to obtain the non-inertial equations. Again, we consider that the parameter $\sigma^m \to 0$, so that the functional is now

$$F[u, \mathbf{m}] \equiv \int_\Omega f(u, \mathbf{m})\, dV, \tag{4.33}$$

with the corresponding Hamiltonian

$$H[u, \mathbf{m}] \equiv \int_\Omega \left(\frac{1}{2} u \cdot u + W + \psi_m\right) dV. \tag{4.34}$$

Analogously to §3.2, we use the transformation

$$\frac{\delta H}{\delta(\sigma^m \dot{m}_{\alpha\beta})} = \dot{m}_{\alpha\beta} = m_{\alpha\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta H}{\delta u_\beta} + m_{\beta\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta H}{\delta u_\alpha}, \tag{4.35}$$

(for arbitrary F and G) corresponding to the upper-convected time derivative, to arrive at the following materially-objective Poisson bracket from the previous bracket, (4.12):

$$\begin{aligned}
\{F, G\} = &- \int_\Omega u_\alpha \left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta u_\alpha} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta u_\alpha}\right) dV \\
&- \int_\Omega m_{\alpha\beta}\left(\frac{\delta F}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta G}{\delta m_{\alpha\beta}} - \frac{\delta G}{\delta u_\gamma}\frac{\partial}{\partial r_\gamma}\frac{\delta F}{\delta m_{\alpha\beta}}\right) dV \\
&- \int_\Omega m_{\alpha\gamma}\left(\frac{\partial}{\partial r_\gamma}\left(\frac{\delta F}{\delta u_\beta}\right)\frac{\delta G}{\delta m_{\alpha\beta}} - \frac{\partial}{\partial r_\gamma}\left(\frac{\delta G}{\delta u_\beta}\right)\frac{\delta F}{\delta m_{\alpha\beta}}\right) dV \\
&- \int_\Omega m_{\beta\gamma}\left(\frac{\partial}{\partial r_\gamma}\left(\frac{\delta F}{\delta u_\alpha}\right)\frac{\delta G}{\delta m_{\alpha\beta}} - \frac{\partial}{\partial r_\gamma}\left(\frac{\delta G}{\delta u_\alpha}\right)\frac{\delta F}{\delta m_{\alpha\beta}}\right) dV \\
&+ 2\int_\Omega m_{\gamma\varepsilon} m_{\alpha\beta}\left(\frac{\partial}{\partial r_\beta}\left(\frac{\delta F}{\delta u_\alpha}\right)\frac{\delta G}{\delta m_{\gamma\varepsilon}} - \frac{\partial}{\partial r_\beta}\left(\frac{\delta G}{\delta u_\alpha}\right)\frac{\delta F}{\delta m_{\gamma\varepsilon}}\right) dV.
\end{aligned} \tag{4.36}$$

The dissipation bracket corresponding to Equation (3.30) is

$$[F, G] \equiv \int_\Omega R^m_{\alpha\beta\gamma\varepsilon} \frac{\partial}{\partial r_\alpha}\left(\frac{\delta F}{\delta u_\beta}\right) \frac{\partial}{\partial r_\gamma}\left(\frac{\delta G}{\delta u_\varepsilon}\right) dV + \int_\Omega P^m_{\alpha\beta\gamma\varepsilon} \frac{\delta F}{\delta m_{\alpha\beta}} \frac{\delta G}{\delta m_{\gamma\varepsilon}} dV$$

$$+ \int_\Omega L^m_{\alpha\beta\gamma\varepsilon}\left(\frac{\partial}{\partial r_\alpha}\left(\frac{\delta F}{\delta u_\beta}\right)\frac{\delta G}{\delta m_{\gamma\varepsilon}} - \frac{\partial}{\partial r_\alpha}\left(\frac{\delta G}{\delta u_\beta}\right)\frac{\delta F}{\delta m_{\gamma\varepsilon}}\right) dV$$

$$- \int_\Omega L^m_{\eta\zeta\gamma\gamma} m_{\alpha\beta}\left(\frac{\partial}{\partial r_\eta}\left(\frac{\delta F}{\delta u_\zeta}\right)\frac{\delta G}{\delta m_{\alpha\beta}} - \frac{\partial}{\partial r_\eta}\left(\frac{\delta G}{\delta u_\zeta}\right)\frac{\delta F}{\delta m_{\alpha\beta}}\right) dV, \quad (4.37)$$

where

$$\begin{aligned} R^m_{\alpha\beta\gamma\varepsilon} \equiv {} & \beta^m_1(m_{\alpha\gamma}m_{\beta\varepsilon} + m_{\alpha\varepsilon}m_{\beta\gamma})/2 + \beta^m_4(\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\alpha\varepsilon}\delta_{\beta\gamma})/2 \\ & + \beta^m_2(\delta_{\alpha\varepsilon}m_{\beta\gamma} + \delta_{\beta\varepsilon}m_{\alpha\gamma} + \delta_{\alpha\gamma}m_{\beta\varepsilon} + \delta_{\beta\gamma}m_{\alpha\varepsilon})/2 \\ & + \beta^m_3(m_{\beta\zeta}m_{\zeta\varepsilon}\delta_{\alpha\gamma} + m_{\alpha\zeta}m_{\zeta\varepsilon}\delta_{\beta\gamma} + m_{\beta\zeta}m_{\zeta\gamma}\delta_{\alpha\varepsilon} + m_{\alpha\zeta}m_{\zeta\gamma}\delta_{\beta\varepsilon})/2 \\ & + \beta^m_5(m_{\alpha\zeta}m_{\zeta\gamma}m_{\beta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}m_{\beta\gamma} + m_{\alpha\gamma}m_{\beta\zeta}m_{\zeta\varepsilon} + m_{\alpha\varepsilon}m_{\beta\zeta}m_{\zeta\gamma})/2 \\ & + \beta^m_6(m_{\alpha\zeta}m_{\zeta\gamma}m_{\beta\eta}m_{\eta\varepsilon} + m_{\alpha\zeta}m_{\zeta\varepsilon}m_{\beta\eta}m_{\eta\gamma})/2 \end{aligned} \quad (4.38a)$$

$$P^m_{\alpha\beta\gamma\varepsilon} \equiv \frac{1}{\beta^m_7}\left[(\delta_{\alpha\varepsilon}\delta_{\beta\gamma} + \delta_{\beta\varepsilon}\delta_{\alpha\gamma})/2 + 3m_{\alpha\beta}m_{\gamma\varepsilon}\right], \quad (4.38b)$$

and

$$L^m_{\alpha\beta\gamma\varepsilon} \equiv \frac{1}{2}(\beta^m_8 - 1)(\delta_{\alpha\varepsilon}m_{\beta\gamma} + \delta_{\beta\varepsilon}m_{\alpha\gamma} + \delta_{\alpha\gamma}m_{\beta\varepsilon} + \delta_{\beta\gamma}m_{\alpha\varepsilon}), \quad (4.38c)$$

where we have chosen $\mathbf{P}^m$ so as to suit the form of Equation (4.24) when $\sigma^m \rightarrow 0$. Note that the fourth integral in the above dissipation bracket was obtained by applying the mapping (4.10) via Equation (4.11) to the unconstrained dissipation bracket (not shown) in a similar fashion to the preceding cases. (Again, see Appendix B for a discussion concerning the minus signs in the third and fourth terms in the dissipation bracket). In the unit vector description, the unconstrained and constrained dissipation brackets were the same, as was shown for the Poisson brackets. Also, it is now evident from the form of the dissipation[12] that β^m_7 plays the role of the system relaxation time and that β_8^m expresses the degree of non-affine motion. In order to be consistent with the inertial theory of §4.1, it is obvious that

$$\beta_7^m = \alpha_3^m - \alpha_2^m \quad \text{and} \quad \frac{\alpha_3^m}{(\alpha_2^m - \alpha_3^m)} = (\beta_8^m - 1)/2. \tag{4.39}$$

The conditions on the β_i^n of Equation (3.34) probably still apply to the β_i^m of Equation (4.38), but only as necessary and not sufficient conditions.

Using the dynamical equation for F, Equation (4.5), the brackets (4.36, 37), and the functional derivatives (4.18a, b), we can arrive at the evolution equations for the variables u and $\mathbf{m}$:

$$\dot{u}_\alpha = F_\alpha^m - P_{,\alpha} - \left(m_{\gamma\varepsilon,\alpha}\frac{\partial W}{\partial m_{\gamma\varepsilon,\beta}}\right)_{,\beta} + T^m_{\alpha\beta,\beta}, \tag{4.40a}$$

and

$$\begin{aligned}\dot{m}_{\alpha\beta} = {} & \frac{1}{(\alpha_2^m - \alpha_3^m)}\left(\frac{\delta H}{\delta m_{\alpha\beta}} + 3m_{\gamma\varepsilon}\frac{\delta H}{\delta m_{\gamma\varepsilon}}\left(m_{\alpha\beta} - \frac{1}{3}\delta_{\alpha\beta}\right)\right) \\ & + \frac{\alpha_2^m}{(\alpha_2^m - \alpha_3^m)}[m_{\alpha\gamma}u_{\beta,\gamma} + m_{\beta\gamma}u_{\alpha,\gamma}] + \frac{\alpha_3^m}{(\alpha_2^m - \alpha_3^m)} \\ & \cdot [m_{\alpha\gamma}u_{\gamma,\beta} + m_{\beta\gamma}u_{\gamma,\alpha}] \\ & - 2\frac{(\alpha_2^m + \alpha_3^m)}{(\alpha_2^m - \alpha_3^m)}m_{\alpha\beta}m_{\gamma\varepsilon}u_{\gamma,\varepsilon}.\end{aligned} \tag{4.40b}$$

In the above evolution equations, the extra stress is defined as

$$\begin{aligned}T^m_{\alpha\beta} \equiv {} & R^m_{\beta\alpha\gamma\varepsilon}A_{\gamma\varepsilon} + \frac{2\alpha_2^m}{(\alpha_2^m - \alpha_3^m)}m_{\beta\gamma}\frac{\delta H}{\delta m_{\gamma\alpha}} + \frac{2\alpha_3^m}{(\alpha_2^m - \alpha_3^m)}m_{\alpha\gamma}\frac{\delta H}{\delta m_{\gamma\beta}} \\ & - 2\frac{(\alpha_2^m + \alpha_3^m)}{(\alpha_2^m - \alpha_3^m)}m_{\alpha\beta}m_{\gamma\varepsilon}\frac{\delta H}{\delta m_{\gamma\varepsilon}}.\end{aligned} \tag{4.41}$$

The above equations, (4.40, 41), can also be obtained directly from the inertial theory, Equations (4.19–23), in the limit of $\sigma^m \to 0$. In order to verify this statement, one must realize that the $\dot{w}_{\alpha\beta}$ in Equation (4.21) vanishes in the non-inertial limit, and then solve this equation for $w_{\alpha\beta}/\sigma^m$. Substituting the resulting expression into Equation (4.20) then yields the evolution equation for $\dot{m}_{\alpha\beta}$, (4.40b). Substituting $w_{\alpha\beta}/\sigma^m$ into Equation (4.23) then gives the extra-stress expression, (4.41), provided we set

$$\beta_1^m = \alpha_1^m + \frac{8\alpha_2^m\alpha_3^m}{(\alpha_2^m - \alpha_3^m)}, \qquad \beta_4^m = \alpha_4^m, \qquad \beta_5^m = \alpha_7^m,$$

$$\beta_6^m = \alpha_8^m, \qquad \beta_2^m = \alpha_2^m, \quad \text{and} \quad \beta_3^m = \frac{4\alpha_2^m\alpha_3^m}{(\alpha_2^m - \alpha_3^m)} + \alpha_6^m. \tag{4.42}$$

The above evolution equations provide the generalized theory for the non-inertial system. For the special case of $\mathbf{m} = nn$, one can again show that the non-inertial LE theory is recovered, provided that the α_i^m are suitably defined as functions of the α_i, as given by Equation (4.26). Once again, one must also use the constraint (4.31).

5. DISCUSSION

In this paper the generalized bracket formulation has been used in order to systematically generate models for liquid-crystalline flow behavior at various levels of abstraction. The derivations of the above models, performed in the preceding sections using the bracket techniques, was straightforward, albeit very tedious algebraically. The most important outcome of this investigation is the two consistent systems of equations developed for both the inertial and the non-inertial cases, Equations (4.19, 23, 24) and Equations (4.39–41), respectively. All previously derived models (LE theory and the Ericksen scalar-vector theory) were shown to be subcases of this general tensorial theory. In addition, we have succeeded in demonstrating the underlying Hamiltonian structure of the entire hierarchy of dynamical liquid-crystalline equations.

The above generalized theory in terms of the structural tensor, $\mathbf{m}$, has several advantages over the existing rheological theories for liquid crystals. Firstly, the use of the tensor $\mathbf{m}$ allows generalization to biaxial liquid-crystalline systems, which occur frequently and are also of experimental interest.[6] Also, the physics of the isotropic/liquid-crystalline and liquid-crystalline/liquid-crystalline phase transitions can now be explored in a rheological context through the inclusion in the Hamiltonian in Equation (4.6) of the bulk (Landau-de Gennes-type) free energy, H_b, Equation (4.3), which is known to adequately describe the qualitative behavior of phase transitions under no-flow conditions.[6,9,13,14,23,24] In fact, H_b can be incorporated directly into both inertial and non-inertial theories simply by reevaluating the functional derivative $\delta H^n/\delta\mathbf{m}$ with $H^n = H + H_b$:

$$\frac{\delta H^n}{\delta m_{\alpha\beta}} = -\frac{1}{2}\chi_a\left(H_\alpha H_\beta - \frac{1}{3}\delta_{\alpha\beta}H_\gamma H_\gamma\right) - b_1 m_{\alpha\beta,\gamma,\gamma}$$

$$- b_2\left(\frac{1}{2}m_{\beta\gamma,\alpha} + \frac{1}{2}m_{\alpha\gamma,\beta} - \frac{1}{3}\delta_{\alpha\beta}m_{\gamma\varepsilon,\varepsilon}\right)_{,\gamma}$$

$$+ 2a_2\left(m_{\alpha\beta} - \frac{1}{3}\delta_{\alpha\beta}\right) + 3a_3\left(m_{\alpha\gamma}m_{\gamma\beta} - \frac{1}{3}\delta_{\alpha\beta}m_{\gamma\varepsilon}m_{\gamma\varepsilon}\right)$$

$$+ 4a_4\left(m_{\alpha\gamma}m_{\gamma\varepsilon}m_{\varepsilon\beta} - \frac{1}{3}\delta_{\alpha\beta}m_{\gamma\varepsilon}m_{\varepsilon\eta}m_{\eta\gamma}\right). \tag{5.1}$$

In References 13 and 14, a generalized Doi model was introduced using the generalized bracket formulation, which incorporated into the Doi-type, quasi-steady-state theory the effects of the distortion energy, W, as well as the translational diffusivity of the molecules. This theory is easily seen to be a special case of the quasi-steady-state (non-inertial) theory of §4.2. In fact, by setting $\alpha_3^m = 0$, $\mathbf{R}^m = 0$, $\mathbf{L}^m = 0$, and

$$P^m_{\alpha\beta\gamma\varepsilon} = \Lambda(\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\alpha\varepsilon}\delta_{\beta\gamma})/2. \tag{5.2}$$

where Λ is the rotational diffusivity of Doi,[9] the equations of Reference 13 are immediately recovered (except for the translational diffusivity). Thus we come full-circle, finally, in reconciling the two theories, Doi and LE, which once seemed so far apart.

Recently, researchers have made claims that the Doi theory in terms of the distribution function allows tumbling in shear flow,[26] as does the LE theory, although the tumbling phenomenon is lost in making the transition to the order-parameter Doi theory. The Doi decoupling approximation[9] has been blamed for this discrepancy. The theory of §4.2 clearly makes this shear-induced tumbling of the molecular axis possible as a consequence of the more-physically-appealing non-affine motion. Whether or not the tumbling phenomenon at the molecular level, which is based on the assumption of the establishment of a homogeneous shearing motion, is important to the description of the flow behavior of real fluids which have a multidomain inhomogeneous structure remains to be seen.

From the form of the dissipation brackets in both of the above non-inertial theories, and the resulting equations, it is apparent that the non-affine motion has the characteristics of the mixed-convective derivative originally proposed by Gordon and Schowalter.[27] (This is not surprising since these authors used Ericksen's anisotropic fluid theory[1] to derive the form for this mixed derivative). In fact, by setting

$$a = \beta_8^m = 1 + \frac{2\alpha_3^m}{(\alpha_2^m - \alpha_3^m)}, \tag{5.3}$$

where a is the derivative coefficient, we can immediately recast Equations 4.40, 41) into the mixed-derivative equations. When $\alpha_3^m = 0$, $a = 1$ and the upper-convected derivative results; when $\alpha_2^m = 0$, $a = -1$ and we get the lower-convected derivative.

In the continuum approach of this paper, the form of the final evolution equation for $\mathbf{m}$ is directly related to the dissipation tensor of Equation (4.38b). Alternatively, when making the transition from the distribution function theory to the order-parameter theory (Doi-type theories), one usually makes a guess as to the appropriate decoupling approximation. This is akin to 'guessing' a form for the dissipation tensor of Equation (4.38b). Now, however, we realize a criterion that this decoupling approximation must meet: it must be consistent with the inertial theory. Also note that the form of the dissipation is highly dependent on the number and the nature of the variables of the formulation. Characteristically, whereas the influence of the Hamiltonian on the evolution equation for n is affected through the Poisson bracket in the inertial approximation, in the non-inertial one it is obtained through the dissipation. We believe that this phenomenon is a more general one and indicative of the character of the dissipation bracket in the formulation: with this bracket, we try to describe the effects of the non-resolved degrees of freedom. Therefore, when one degree of freedom is allowed to equilibrate (in the inertial case: $\sigma = 0$) part of the effect that it has on the other variables is passed through new terms in the dissipation bracket (compare Equations 3.14 and 3.30).

Currently, a stability analysis upon the equations of §4.2 is underway in order to determine the exact behavior of the solutions to the generalized, quasi-steady-state (non-inertial) theory in shear flow.[30] (Calderer[17,28] has recently done this for a special case of the scalar-vector description, presented in Appendix A, with interesting results.) Also, a numerical procedure is being developed in order to investigate the influence of spatial anisotropy on the shear-flow properties.[30] This model, being formulated in terms of the tensor $\mathbf{m}$, should be, in principle, not more difficult to be used in numerical calculations than any standard viscoelastic flow model (e.g., upper convected Maxwell) for artitrary kinematics. From a continuum mechanics viewpoint the theory is completely general (when the translational diffusivity of Reference 13 is incorporated), and should allow consistent results to be obtained with respect to any other continuum theory involving up to one tensorial structural parameter. Hopefully, the work which is being performed on this system of equations will finally provide some meaningful answers to some long-posed questions in this field.

APPENDIX A

In this appendix, we wish to show how the recent theory of Ericksen[16] (a particular case of which was examined by Calderer)[17,18] can arise as a special case of the tensorial theory of §4. The non-inertial Ericksen scalar-vector theory involves two internal structural parameters: a scalar order parameter, s, describing the spread or distribution of the orientation, and a unit vector, the director n, similar to the one present in the LE theory as discussed before in §2. For $s = 1$, perfect alignment is assumed, with random alignment corresponding to $s = 0$. Two evolution equations are provided,[16] for s and n:

$$\dot{s} = -\frac{1}{\hat{\beta}_2(s)}\frac{\delta H}{\delta s} - \frac{\hat{\beta}_1(s)}{\hat{\beta}_2(s)}\, n^T \cdot \mathbf{A} \cdot n \qquad \text{(A.1)}$$

and

$$\dot{n} = \Omega \cdot n + \frac{\hat{\gamma}_2(s)}{\hat{\gamma}_1(s)}[n(n^T \cdot \mathbf{A} \cdot n) - \mathbf{A} \cdot n] - \frac{1}{\hat{\gamma}_1(s)} \frac{\delta H}{\delta n}. \tag{A.2}$$

The stress is expressed as

$$\begin{aligned} t'_{\alpha\beta} + p\delta_{\alpha\beta} = {} & \hat{\alpha}_1(s) n_\alpha n_\beta n_\gamma n_\varepsilon A_{\gamma\varepsilon} + \hat{\alpha}_2(s)[\dot{n}_\alpha n_\beta - \Omega_{\alpha\gamma} n_\gamma n_\beta] \\ & + \hat{\alpha}_3(s)[\dot{n}_\beta n_\alpha - \Omega_{\beta\gamma} n_\gamma n_\alpha] \\ & + \hat{\alpha}_4(s) A_{\alpha\beta} + \hat{\alpha}_5(s) n_\beta n_\gamma A_{\gamma\alpha} + \hat{\alpha}_6(s) n_\alpha n_\gamma A_{\gamma\beta} \\ & + \hat{\beta}_1(s) \dot{s} n_\alpha n_\beta - n_{\gamma,\alpha} \frac{\partial W}{\partial n_{\gamma,\beta}} - s_{,\alpha} \frac{\partial W}{\partial s_{,\beta}}, \end{aligned} \tag{A.3}$$

where $\hat{\gamma}_1 = \hat{\alpha}_3 - \hat{\alpha}_2$ and $\hat{\gamma}_2 = \hat{\alpha}_6 - \hat{\alpha}_5 = \hat{\alpha}_2 + \hat{\alpha}_3$.

The above theory involves seven parameters (excluding H), as general functions of s, which we can also see by rewriting the stress Equation (A.3), using Equations (A.1, 2) to substitute for $\dot{n}$ and $\dot{s}$:

$$\begin{aligned} t'_{\alpha\beta} + p\delta_{\alpha\beta} = {} & \hat{\alpha}_4 A_{\alpha\beta} + \left(\hat{\alpha}_1 + \frac{\hat{\gamma}_2^2}{\hat{\gamma}_1} - \frac{\hat{\beta}_1^2}{\hat{\beta}_2}\right) n_\alpha n_\beta n_\gamma n_\varepsilon A_{\gamma\varepsilon} \\ & + \left(\hat{\alpha}_5 - \hat{\alpha}_2 \frac{\hat{\gamma}_2}{\hat{\gamma}_1}\right)[n_\alpha n_\gamma A_{\gamma\beta} + n_\beta n_\gamma A_{\gamma\alpha}] \\ & - \frac{\hat{\beta}_1}{\hat{\beta}_2} n_\alpha n_\beta \frac{\delta H}{\delta s} - s_{,\alpha} \frac{\partial W}{\partial s_{,\beta}} - n_{\gamma,\alpha} \frac{\partial W}{\partial n_{\gamma,\beta}} - \frac{1}{2} \frac{\hat{\gamma}_2}{\hat{\gamma}_1} \\ & \cdot \left[n_\alpha \frac{\delta H}{\delta n_\beta} + n_\beta \frac{\delta H}{\delta n_\alpha}\right] - \frac{1}{2}\left[n_\alpha \frac{\delta H}{\delta n_\beta} - n_\beta \frac{\delta H}{\delta n_\alpha}\right]. \end{aligned} \tag{A.4}$$

From Equations (A.1, 2, 4), we see that there are seven independent parameters are $\hat{\beta}_1$, $\hat{\beta}_2$, $\hat{\gamma}_1$, $\hat{\gamma}_2$, $\hat{\alpha}_4$, $\hat{\alpha}_1$, and $\hat{\alpha}_5$.

In the following, we shall show that one can obtain the above scalar-vector theory from the tensorial theory developed in §4 under the uniaxial approximation

$$m_{\alpha\beta} = s n_\alpha n_\beta + \frac{1-s}{3} \delta_{\alpha\beta}, \tag{A.5a}$$

which implies

$$m_{\alpha\beta,\gamma} = s_{,\gamma}\left(n_\alpha n_\beta - \frac{1}{3}\delta_{\alpha\beta}\right) + s(n_{\alpha,\gamma} n_\beta + n_\alpha n_{\beta,\gamma}), \tag{A.5b}$$

and

$$\dot{m}_{\alpha\beta} = \dot{s}\left(n_\alpha n_\beta - \frac{1}{3}\delta_{\alpha\beta}\right) + s(\dot{n}_\alpha n_\beta + n_\alpha \dot{n}_\beta). \tag{A.5c}$$

Using differentiation by parts, we have

$$\frac{\delta H}{\delta n_\alpha} = 2s\left(\frac{\delta H}{\delta m_{\alpha\gamma}} n_\gamma - \frac{\delta H}{\delta m_{\gamma\beta}} n_\beta n_\gamma n_\alpha\right), \tag{A.6a}$$

$$\frac{\delta H}{\delta s} = \frac{\delta H}{\delta m_{\alpha\beta}} n_\alpha n_\beta, \tag{A.6b}$$

and

$$\frac{\delta W}{\delta n_{\gamma,\beta}} = 2s\frac{\partial W}{\partial m_{\gamma\varepsilon,\beta}} n_\varepsilon \quad \text{and} \quad \frac{\partial W}{\partial s_{,\beta}} = \frac{\partial W}{\partial m_{\gamma\varepsilon,\beta}} n_\varepsilon n_\gamma. \tag{A.6c}$$

Substitution of the identities (A.5, 6) into Equation (4.40b) and double-dotting with nn yields the evolution equation for the scalar order parameter:

$$\dot{s} = \frac{3}{2}\frac{1+2s^2}{(\alpha_2^m - \alpha_3^m)}\frac{\delta H}{\delta s} + \frac{(\alpha_2^m + \alpha_3^m)}{(\alpha_2^m - \alpha_3^m)}(2s+1)(1-s)n_\beta n_\gamma A_{\beta\gamma}. \tag{A.7}$$

Again substituting identities (A.5, 6) into Equation (4.40b), but this time dotting with n and then substituting (A.7) gives

$$\dot{n} = \Omega \cdot n - \frac{(\alpha_2^m + \alpha_3^m)}{(\alpha_2^m - \alpha_3^m)}\frac{2+s}{3s}[n(n^T \cdot \mathbf{A} \cdot n) - \mathbf{A} \cdot n] + \frac{1}{(\alpha_2^m - \alpha_3^m)}\frac{1}{2s^2}\frac{\delta H}{\delta n_\alpha}. \tag{A.8}$$

Using Equations (A.5a, 6) in Equations (4.40a, 41) produces the constitutive equation for the stress:

$$\begin{aligned}\Pi_{\alpha\beta} = {} & \beta_1^m s^2 n_\alpha n_\beta n_\gamma n_\varepsilon A_{\gamma\varepsilon} + \left(\beta_1^m s\frac{1-s}{3} + \beta_2^m s + \beta_3^m s\frac{s+2}{3}\right) \\ & \cdot (n_\alpha n_\gamma A_{\gamma\beta} + n_\beta n_\gamma A_{\alpha\gamma}) \\ & + \left[\beta_4^m + \frac{2}{3}\beta_2^m(1-s) + \frac{2}{9}\beta_3^m(1-s)^2 + \frac{1}{9}\beta_1^m(1-s)^2\right]A_{\alpha\beta} \\ & - s_{,\alpha}\frac{\partial W}{\partial s_{,\beta}} - n_{\gamma,\alpha}\frac{\partial W}{\partial n_{\gamma,\beta}} + \frac{(\alpha_2^m + \alpha_3^m)}{(\alpha_2^m - \alpha_3^m)}(1-s)(2s+1)\frac{\delta H}{\delta s}n_\alpha n_\beta \\ & + K'\delta_{\alpha\beta} + \frac{1}{2}\frac{2+s}{3s}\frac{(\alpha_2^m + \alpha_3^m)}{(\alpha_2^m - \alpha_3^m)}\left[n_\alpha\frac{\delta H}{\delta n_\beta} + n_\beta\frac{\delta H}{\delta n_\alpha}\right] \\ & - \frac{1}{2}\left[n_\alpha\frac{\delta H}{\delta n_\beta} - n_\beta\frac{\delta H}{\delta n_\alpha}\right],\end{aligned} \tag{A.9}$$

provided that one uses the constraint

$$\frac{2}{3}\frac{\delta H}{\delta m_{\alpha\beta}} = \left(n_\alpha n_\beta - \frac{1}{3}\delta_{\alpha\beta}\right)\frac{\delta H}{\delta s} + \frac{1}{3s}\left[n_\alpha \frac{\delta H}{\delta n_\beta} + n_\beta \frac{\delta H}{\delta n_\alpha}\right] \tag{A.10}$$

to restrict the excess information contained in the tensorial theory. Note that this constraint is entirely consistent with the definitions (A.6a, b). In Equation (A.9), K' is an isotropic function of H which can be incorporated into the pressure, and $\beta_5^m = \beta_6^m = 0$ (solely for convenience).

In order to see how the constraint (A.10) arises, we must consider the lowest-order weighted-residual approximation to $\delta H/\delta \mathbf{m}$. Starting with

$$\frac{\delta m_{\alpha\beta}}{\delta m_{\gamma\delta}} = \frac{\partial m_{\alpha\beta}}{\partial s}\frac{\delta s}{\delta m_{\gamma\delta}} + \frac{\partial m_{\alpha\beta}}{\partial n_\varepsilon}\frac{\delta n_\varepsilon}{\delta m_{\gamma\delta}} = \frac{1}{2}(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}) - \frac{1}{3}\delta_{\gamma\delta}\delta_{\alpha\beta}, \tag{A.11}$$

we realize that we have more equations than unknowns, and thus an over-determinate system. We therefore seek the best approximation, using the weighted-residuals method, by taking weighted averages of the above equation provided by double-dotting (A.11) with δ and dotting with n. We obtain respectively

$$\frac{\partial m_{\alpha\alpha}}{\partial s}\frac{\delta s}{\delta m_{\gamma\delta}} + \frac{\partial m_{\alpha\alpha}}{\partial n_\varepsilon}\frac{\delta n_\varepsilon}{\delta m_{\gamma\delta}} = 0$$

and

$$n_\beta\frac{\partial m_{\alpha\beta}}{\partial s}\frac{\delta s}{\delta m_{\gamma\delta}} + n_\beta\frac{\partial m_{\alpha\beta}}{\partial n_\varepsilon}\frac{\delta n_\varepsilon}{\delta m_{\gamma\delta}} = \frac{1}{2}(\delta_{\alpha\gamma}n_\delta + \delta_{\alpha\delta}n_\gamma) - \frac{1}{3}\delta_{\gamma\delta}n_\alpha. \tag{A.12}$$

Now we have a consistent set of four equations for four unknowns, $\delta n_\alpha/\delta m_{\gamma\delta}$ and $\delta s/\delta m_{\gamma\delta}$ for every partial derivative with respect to $m_{\gamma\delta}$. Using Equation (A.5a), we can calculate $\partial m_{\alpha\beta}/\partial s$ and $\partial m_{\alpha\beta}/\partial n_\varepsilon$, so that we may solve (A.12) to obtain

$$\frac{\delta n_\alpha}{\delta m_{\gamma\delta}} = \frac{1}{2s}(\delta_{\alpha\gamma}n_\delta + \delta_{\alpha\delta}n_\gamma) - \frac{1}{s}n_\alpha n_\gamma n_\delta \tag{A.13}$$

and

$$\frac{\delta s}{\delta m_{\gamma\delta}} = \frac{3}{2}\left(n_\gamma n_\delta - \frac{1}{3}\delta_{\gamma\delta}\right), \tag{A.14}$$

realizing, of course, that these values are the best estimates based on the above-mentioned weighted-residuals procedure. Finally, by using differentiation by parts,

$$\frac{\delta H}{\delta m_{\alpha\beta}} = \frac{\partial H}{\partial s}\frac{\delta s}{\delta m_{\alpha\beta}} + \frac{\partial H}{\partial n_\gamma}\frac{\delta n_\gamma}{\delta m_{\alpha\beta}}, \tag{A.15}$$

we can arrive directly at the constraint (A.10).

By comparing Equations (A.7, 8, 9) to Equations (A.1, 2, 4), we see that the two theories are equivalent provided the following relationships hold:

$$\hat{\beta}_2 = -2\frac{(\alpha_2^m - \alpha_3^m)}{3 + 6s^2}, \qquad \frac{\hat{\beta}_1}{\hat{\beta}_2} = -\frac{(\alpha_2^m + \alpha_3^m)}{(\alpha_2^m - \alpha_3^m)}(2s + 1)(1 - s),$$

$$\hat{\alpha}_4 = \beta_4^m + \frac{2}{3}\beta_2^m(1 - s) + \frac{2}{9}\beta_3^m(1 - s)^2 + \frac{1}{9}\beta_1^m(1 - s)^2,$$

$$\left(\hat{\alpha}_1 + \frac{\hat{\gamma}_2^2}{\hat{\gamma}_1} - \frac{\hat{\beta}_1^2}{\hat{\beta}_2}\right) = \beta_1^m s^2, \qquad \frac{\hat{\gamma}_2}{\hat{\gamma}_1} = -\frac{(\alpha_2^m + \alpha_3^m)}{(\alpha_2^m - \alpha_3^m)}\frac{2 + s}{3s},$$

and

$$\hat{\alpha}_5 - \hat{\alpha}_2\frac{\hat{\gamma}_2}{\hat{\gamma}_1} = \beta_1^m s\frac{1 - s}{3} + \beta_2^m s + \beta_3^m s\frac{s + 2}{3}, \qquad \hat{\gamma}_1 = 2s^2(\alpha_3^m - \alpha_2^m). \tag{A.16}$$

Inclusion of non-zero β_5^m and/or β_6^m modifies trivially the right-hand side of the third, fourth and sixth of the above equations. The important observation, however, is that by dividing $\hat{\beta}_1/\hat{\beta}_2$ by $\hat{\gamma}_2/\hat{\gamma}_1$, we always get the constraint

$$\frac{\hat{\beta}_1}{\hat{\beta}_2}\frac{\hat{\gamma}_1}{\hat{\gamma}_2} = 3s\frac{(2s + 1)(1 - s)}{(2 + s)}, \tag{A.17}$$

which reduces the number of independent parameters in the Ericksen theory from seven to six. The underlying physical meaning behind this constraint is that the dependencies of the time variations of s and n on $\mathbf{A}$ are correlated since they arise from a single evolution equation for $\mathbf{m}$.

Ericksen's theory has been derived here in its non-inertial form. It is obvious that the same substitutions (A.5, 6) can be used in conjunction with the theory of §4.1 to develop the inertial scalar-vector theory.

APPENDIX B

The objective of this appendix is to rationalize the form of the dissipation bracket used in this work. Note that in this appendix, we choose to work in terms of the tensorial representation, although the same arguments apply to the unit-vector description as well.

The dissipation bracket couples the tensors (affinities) $\nabla(\delta H/\delta u)$ and $\delta H/\delta \mathbf{m}$ with themselves and each other. The lowest possible order is biquadratic in $\nabla(\delta H/\delta u)$

and $\delta H/\delta \mathbf{m}$, and therefore the (unconstrained) bracket is written explicitly as

$$[F, G] \equiv \int_\Omega \left(R^{ab}_{\alpha\beta\gamma\varepsilon} \nabla_\alpha \left(\frac{\delta F}{\delta u_\beta}\right) \nabla_\gamma \left(\frac{\delta G}{\delta u_\varepsilon}\right) + R^{ba}_{\alpha\beta\gamma\varepsilon} \nabla_\alpha \left(\frac{\delta G}{\delta u_\beta}\right) \nabla_\gamma \left(\frac{\delta F}{\delta u_\varepsilon}\right)\right) dV$$

$$+ \int_\Omega \left(P^{ab}_{\alpha\beta\gamma\varepsilon} \frac{\delta F}{\delta m_{\alpha\beta}} \frac{\delta G}{\delta m_{\gamma\varepsilon}} + P^{ba}_{\alpha\beta\gamma\varepsilon} \frac{\delta G}{\delta m_{\alpha\beta}} \frac{\delta F}{\delta m_{\gamma\varepsilon}}\right) dV$$

$$+ \int_\Omega \left(L^{ab}_{\alpha\beta\gamma\varepsilon} \nabla_\alpha \left(\frac{\delta F}{\delta u_\beta}\right) \frac{\delta G}{\delta m_{\gamma\varepsilon}} + L^{ba}_{\alpha\beta\gamma\varepsilon} \nabla_\alpha \left(\frac{\delta G}{\delta u_\beta}\right) \frac{\delta F}{\delta m_{\gamma\varepsilon}}\right) dV. \quad \text{(B.1)}$$

We can relate the phenomenological coefficient matrices, however, using the Onsager-Casimir reciprocal relations for a general matrix $\mathbf{Z}$:

$$\mathbf{Z}^{ab}(\tau) = \eta_a \eta_b \mathbf{Z}^{ba}(-\tau), \quad \text{(B.2)}$$

where η_a and η_b are the parities of each affinity ($\nabla(\delta H/\delta u)$ and $\delta H/\delta \mathbf{m}$) under a microscopic time reversal,[29] indicated by τ. The parity of $\nabla(\delta H/\delta u)$ is -1, and the parity of $\delta H/\delta \mathbf{m}$ is 1. Hence,

$$\mathbf{R}^{ab} = \mathbf{R}^{ba}, \qquad \mathbf{P}^{ab} = \mathbf{P}^{ba}, \quad \text{and} \quad \mathbf{L}^{ab} = -\mathbf{L}^{ba}. \quad \text{(B.3)}$$

Thus we arrive at the bracket as given by Equation (4.37).

Since the term involving the cross-coupling is antisymmetric, it does not contribute to the overall entropy production. It is included in the dissipation bracket rather than an additional contribution to the Poisson bracket of Equation (4.36) since the resulting bracket then loses its symplectic nature (i.e., it does not satisfy the Jacobi identity).[12] Following Woods,[29] it is known that for couplings with $\eta_a\eta_b = -1$, if $\mathbf{Z}^{ab}(\tau) = \mathbf{Z}^{ba}(-\tau)$ (which is the case for $\mathbf{L}$), the process makes no contribution to the entropy production. This represents a well-founded thermodynamic principle concerning dissipative systems.

APPENDIX C

Both Leslie[5] and Parodi[20] have performed the calculation of determining the constraints on the α_i, but neither have been very extroverted in their expositions on this subject. In the following, we show briefly how this calculation may be performed for the case of Equation (3.16), and we arrive at the constraints imposed by Leslie.[5] These constraints are slightly different than those of Parodi[20]; the discrepancy being possibly due to the neglect of the constraints on $\mathbf{A}$ and N by Parodi.

For an incompressible fluid, $\mathbf{A}$ is both symmetric and traceless:

$$A_{\alpha\beta} = \frac{1}{2}(\hat{A}_{\alpha\beta} + \hat{A}_{\beta\alpha}) - \frac{1}{3}\hat{A}_{\gamma\gamma}\delta_{\alpha\beta}. \quad \text{(C.1)}$$

Also, N must satisfy the constraint

$$N_\alpha - N_\beta n_\beta n_\alpha = 0 \Rightarrow N_\alpha = \hat{N}_\alpha - \hat{N}_\beta n_\beta n_\alpha. \tag{C.2}$$

Directly from Equation (3.16), we can rewrite the inequality as

$$\alpha_1(n_\alpha n_\beta A_{\alpha\beta})^2 + \alpha_4(A_{\alpha\beta})^2 + \eta N_\alpha A_{\alpha\beta} n_\beta + \beta(A_{\alpha\beta} n_\beta)^2 + \gamma_1(N_\alpha)^2 \geq 0, \tag{C.3}$$

where

$$\beta = \alpha_5 + \alpha_6, \tag{C.4}$$

and

$$\eta = \alpha_2 + \alpha_3 + \alpha_6 - \alpha_5. \tag{C.5}$$

Since the coordinate system is completely arbitrary, we can choose our Cartesian coordinates so that the x_1 direction lies in the direction of n_1, so that n may be written as

$$n = (1, 0, 0)^T. \tag{C.6}$$

Substituting Equations (C.1, 2, 6) into inequality (C.3) yields a 9×9 symmetric matrix, $\mathbf{B}$, satisfying the inequality

$$C^T \cdot \mathbf{B} \cdot C \geq 0, \tag{C.7}$$

where C is the vector

$$C \equiv (\hat{A}_{11}, \hat{A}_{22}, \hat{A}_{33}, \hat{A}_{12}, \hat{A}_{23}, \hat{A}_{31}, \hat{N}_1, \hat{N}_2, \hat{N}_3)^T. \tag{C.8}$$

In order for the inequality, (C.7), to be valid, $\mathbf{B}$ must be non-negative definite. The non-zero components of this matrix, $\mathbf{B}$, are

$$B_{11} = \frac{4}{9}(\alpha_1 + \beta) + \frac{2}{3}\alpha_4,$$

$$B_{22} = B_{33} = \frac{1}{9}(\alpha_1 + \beta) + \frac{2}{3}\alpha_4,$$

$$B_{44} = B_{66} = 2\alpha_4 + \beta,$$

$$B_{55} = 2\alpha_4,$$

$$B_{88} = B_{99} = \gamma_1,$$

$$B_{12} = B_{21} = B_{13} = B_{31} = -\frac{2}{9}(\alpha_1 + \beta) - \frac{1}{3}\alpha_4,$$

$$B_{23} = B_{32} = \frac{1}{9}(\alpha_1 + \beta) - \frac{1}{3}\alpha_4,$$

and

$$B_{84} = B_{48} = B_{96} = B_{69} = \eta/2. \tag{C.9}$$

Since **B** must be non-negative definite, all the diagonal components must be greater than or equal to zero, as well as the determinants of all of the principle minors. This easily results in a number of conditions on the α_i, five of which are not superfluous:

$$\alpha_4 \geq 0,$$

$$2\alpha_4 + \beta \geq 0,$$

$$\gamma_1 \geq 0,$$

$$2\alpha_1 + 3\alpha_4 + 2\beta \geq 0,$$

and

$$4\gamma_1(2\alpha_4 + \beta) \geq \eta^2. \tag{C.10}$$

These are the conditions of Leslie (Reference 5, Equation 35).

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