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## Molecular Crystals and Liquid Crystals

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# Nonlocal Continuum Theory of Liquid Crystals

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A nonlocal continuum theory of liquid crystals is constructed to explain and predict the physical behavior of liquid crystals under long range intermolecular forces. Balance laws consist of conservation of mass and microinertia, balance of momenta and energy. Constitutive equations are given for the equilibrium and non-equilibrium parts of the stress, couple stress, free energy, entropy and nonlocal body force and couple. Thermodynamic restrictions and material frame-indifference are studied. The theory is valid for liquid crystals having arbitrary shapes (inertia). Passage is made to the thread-like molecules and to local theory. Applications are considered to two-dimensional problems, steady, plane shear flows and dispersion of twist waves.

## 1 INTRODUCTION

It is well-known that the physical behavior of liquid crystals are affected by distant intermolecular forces and couples, to a significant degree. Particularly, for short time (high frequency) behavior and near rigid boundaries, the nonlocal effects become dominant often superceding the local effects. The nonlocal effects resulting from long range intermolecular forces and short time effects were noted briefly by Oseen<sup>1</sup> and Foster, *et al.*<sup>2</sup> In the case of electromagnetic (E-M) effects, the long range effects are even more important since E-M loads are basically nonlocal in character.

Recent applications of nonlocal elasticity to several problems in fracture mechanics and dislocation theory have shown that atomic and molecular scale phenomena and high frequency behavior of materials can be predicted by means of the nonlocal theory (cf. 3-6). In fact, it can be shown that atomic lattice dynamics is included in the nonlocal theory.<sup>7,8</sup> Encouraged with these calculations, we present here a nonlocal theory for liquid crystals.

Essentials of the theory were elaborated, to some extent, in our work<sup>9</sup> on nonlocal micropolar continuum theory. However, constitutive equations of

nonlocal micropolar fluids developed there must be extended to include the effect of elastic twist ( $\gamma_{kl}$ ) and the variation of anisotropy with the motions of molecular elements. In our previous work on local theory,<sup>10</sup> this latter effect was realized by means of the microinertia tensor  $j_{kl}$  of molecules in motion.

For liquid crystals having arbitrary molecular shapes, a single director is not adequate to encompass material properties and one needs tensorial anisotropy indicator as introduced in Ref. 10. In fact, this prediction is born out, with the discovery of discotic liquid crystals.<sup>11,12</sup> Therefore, here we develop a nonlocal theory of liquid crystals whose molecular elements may be of any shape possessing arbitrary microinertia tensors.

In Section 2, we collect basic kinematical quantities and strain measures. Section 3 gives the balance laws which are the same as those of micropolar continua (cf. 9). Constitutive equations are developed in Section 4, where we explore restrictions arising from invariance requirements under arbitrary rigid motions of the spatial frame reference (objectivity) and the second law of thermodynamics. The general theory so-developed is specialized for the additive functionals in Section 5. In Section 6, we indicate the passage to the director theory which applies to liquid crystals with thread-like elements. The local theory is included in the nonlocal theory when the internal characteristic length (e.g. lattice parameter) approaches to zero (Section 7). In Section 8, we discuss briefly the nature of nonlocal material moduli. Section 9 contains two dimensional problems, steady plane shear flows and dispersion of twist waves.

The field equations of the nonlocal theory are nonlinear integropartial differential equations. Even for simple problems, major difficulties exist in dealing with these equations. However, we believe that nonlocal effects are prominent in boundary layers near rigid walls, around sharp corners and in classically discontinuous flow regimes. Therefore, it should be possible to establish approximate theories, or else proceed with computer aided programs, to tackle these important problems.

## 2 KINEMATICS

In a micropolar continuum, a material point is considered to possess mass density  $\rho$  and a microinertia tensor  $j_{kl}$ . By its presence,  $j_{kl}$  not only controls the rotatory motions of the material points, but also the directional dependence of material properties. The motion of a point is then equivalent to a rigid body motion.

Referred to a set of rectangular coordinates,  $X_K$ ,  $K = 1, 2, 3$ , in the reference state, a material point is characterized by its position vector  $\mathbf{X}$  and a director  $\Xi$  attached to the point. The motion of  $\mathbf{X}$  is described by the following two sets of equations

$$x_k = x_k(\mathbf{X}, t), \quad \xi_k = \chi_{kK}(\mathbf{X}, t) \Xi_K \quad (2.1)$$

of which the first expresses the translatory motions of  $\mathbf{X}$  and the second one its rotations. The repeated indices are summed over 1, 2, 3. The inverse motions are posited to be unique and given by

$$X_K = X_K(\mathbf{x}, t), \quad \Xi_K = \chi_{Kk}^{-1} \xi_k \quad (2.2)$$

where  $\chi_{Kk}^{-1} = \chi_{kK}$  is an orthogonal two-point tensor field so that

$$\begin{aligned} x_{k,K} X_{K,l} &= \delta_{kl}, & X_{K,k} x_{k,L} &= \delta_{KL}, \\ \chi_{kK} \chi_{lK} &= \delta_{kl}, & \chi_{kK} \chi_{kL} &= \delta_{KL} \end{aligned} \quad (2.3)$$

For a fluent body, by considering the relative configuration, at time  $t$ , we have introduced the following strain measures:<sup>10</sup>

$$c_{kl} = X_{K,k} \chi_{lK}, \quad \gamma_{kl} = \frac{1}{2} \epsilon_{kmn} \chi_{mK} \chi_{nK,l} \quad (2.4)$$

and the rate of deformation tensors

$$a_{kl} = v_{l,k} + v_{kl}, \quad b_{kl} = v_{k,l} \quad (2.5)$$

Here,  $v_{kl}$  is the gyration tensor defined by

$$v_{kl} = -\epsilon_{klm} v_m = \dot{\chi}_{kK} \chi_{lK} = -v_{lk} \quad (2.6)$$

with  $\epsilon_{klm}$  being the alternating tensor. Indices following a comma denote partial differentiation and a superposed dot or  $D/Dt$  material time rate, e.g.

$$v_{k,l} = \frac{\partial v_k}{\partial x_l}, \quad x_{k,K} = \frac{\partial x_k}{\partial X_K}, \quad \dot{v}_k = \frac{Dv_k}{Dt} = \frac{\partial v_k}{\partial t} + v_{k,l} v_l, \quad v_k = \frac{\partial x_k(\mathbf{X}, t)}{\partial t} \quad (2.7)$$

We have shown that  $\chi_{kK}$ ,  $\gamma_{kl}$  and  $v_k$  can be expressed in terms of an axial vector  $\phi_k$  and its material time derivative.<sup>13</sup>

$$\chi_{kK} = [\cos \phi \delta_{kl} + (1 - \cos \phi) n_k n_l - \sin \phi \epsilon_{klm} n_m] \delta_{lK}, \quad (2.8)$$

$$\gamma_{kl} = n_k \phi_{,l} + \sin \phi n_{k,l} - (1 - \cos \phi) \epsilon_{kmn} n_m n_{n,l} \quad (2.9)$$

$$v_k = \Lambda_{kl} \dot{\phi}_l \quad (2.10)$$

where

$$\begin{aligned} n_k &= \phi_k / \phi, \quad \phi = (\phi_k \phi_k)^{1/2} \\ \Lambda_{kl} &= \frac{\sin \phi}{\phi} \delta_{kl} + \left(1 - \frac{\sin \phi}{\phi}\right) n_k n_l - \frac{1}{\phi} (1 - \cos \phi) \epsilon_{klm} n_m \end{aligned} \quad (2.11)$$

Here,  $\delta_{kK}$  is the direction cosines between the spatial and material frames. When these frames coincide,  $\delta_{kK}$  becomes Kronecker delta.

We remark that for the continuum description of motions of micropolar bodies, the ultimate desire is to determine the functions  $x_k(\mathbf{X}, t)$  and  $\chi_{kK}(\mathbf{X}, t)$ .

The directors  $\Xi_K$  and  $\xi_k$  are "internal variables," affecting the directional properties of micropolar bodies by means of the microinertia tensor  $j_{kl}$ .

### 3 BALANCE LAWS

The balance laws of a nonlocal micropolar continua were obtained in Ref. 9. For an inert body, these are of the form (in  $\mathcal{V} - \sigma$ ):

Mass

$$\dot{\rho} + \rho v_{k,k} = 0 \quad (3.1)$$

Microinertia

$$\frac{Dj_{kl}}{Dt} - j_{km}v_{lm} - j_{lm}v_{km} = 0 \quad (3.2)$$

Momentum

$$t_{kl,k} + \rho(f_l - \dot{v}_l) + \rho f_l = 0 \quad (3.3)$$

Moment of Momentum

$$m_{kl,k} + \epsilon_{lmn}t_{mn} + \rho(l_l - \dot{\sigma}_l) + \rho(\hat{l}_l - \epsilon_{lmn}x_m f_n) = 0 \quad (3.4)$$

Energy

$$\begin{aligned} -\rho \dot{e} + t_{kl}a_{kl} + m_{kl}b_{lk} + q_{k,k} + \rho h - \rho f_k v_k \\ - \rho(\hat{l}_k - \epsilon_{klm}x_l f_m)v_k + \rho \dot{h} = 0 \end{aligned} \quad (3.5)$$

Entropy

$$\rho \dot{\eta} - \left( \frac{q_k}{\theta} \right)_{,k} - \frac{\rho h}{\theta} - \rho \dot{b} \geq 0 \quad (3.6)$$

where

$\rho$ = mass density	$\dot{\sigma}_k$ = spin inertia
$j_{kl}$ = microinertia tensor	$v_k$ = velocity vector
$t_{kl}$ = stress tensor	$\nu_{kl}$ = gyration tensor
$m_{kl}$ = couple stress tensor	$f_i$ = body force density
$\epsilon$ = internal energy density	$l_i$ = body couple density
$\eta$ = entropy density	$q_k$ = heat vector
$h$ = energy source	$\theta$ = absolute temperature
$f_k$ = nonlocal body force residual	$\hat{l}_i$ = nonlocal body couple residual
$\hat{b}$ = nonlocal entropy residual	$\hat{h}$ = nonlocal energy residual

Equations (3.1) to (3.5) are, respectively, the local balance laws of mass, microinertia, momentum, angular momentum and energy and (3.6) is the ex-

pression of the second law of thermodynamics. The spin inertia  $\dot{\sigma}_k$  is defined by

$$\dot{\sigma}_k = \frac{D}{Dt} (j_{kl} v_l) = j_{kl} v_l - \epsilon_{kmr} j_{lm} v_r v_l \quad (3.7)$$

These laws are valid in the body  $(\mathcal{V} - \sigma)$  with material volume  $\mathcal{V}$  excluding a discontinuity surface  $\sigma$  which may be sweeping the body with its own velocity.

The residuals carrying a hat ( $\hat{\cdot}$ ) are the long-range effects of the distant material points in the body to state of the body at the reference point  $x$ . They are subject to

$$\int_{\mathcal{V}-\sigma} \{\rho \hat{f}, \rho \hat{l}, \rho \hat{h}, \rho \hat{b}\} dv = 0 \quad (3.8)$$

of these,  $\hat{f}$  and  $\hat{l}$ , respectively, represent the long-range gravitational forces, and couples, while  $\hat{h}$  and  $\hat{b}$  the energy and entropy changes caused by the distant points of the body, at  $x$ . Generally,  $\hat{f}$  and  $\hat{l}$  are negligible as compared to applied forces.

Associated with the balance laws (3.1) to (3.6), there exists a set of jump conditions across  $\sigma$  which are not copied here. For these, see Ref. 9, pp. 212, 213.

Upon eliminating  $h$  between (3.5) and (3.6), we obtain the generalized Clausius-Duhem (C-D) inequality:

$$\begin{aligned} -\frac{\rho}{\theta} (\dot{\psi} + \dot{\theta} \eta) + \frac{1}{\theta} t_{kl} a_{kl} + \frac{1}{\theta} m_{kl} b_{lk} + \frac{1}{\theta^2} q_k \theta_{,k} \\ - \frac{\rho}{\theta} f_k v_k - \frac{\rho}{\theta} (l_k - \epsilon_{klm} x_l f_m) v_k + \frac{\rho}{\theta} \dot{h} - \rho \dot{b} \geq 0, \quad \mathcal{V} - \sigma \end{aligned} \quad (3.9)$$

where  $\psi$  is the Helmholtz free energy defined by

$$\psi = \epsilon - \theta \eta \quad (3.10)$$

This inequality is fundamental for the discussion of nonlocal thermodynamics of micropolar bodies.

For future use, we also give the integral form of (3.2), as derived by Eringen:<sup>14</sup>

$$j_{kl} = J_{KL} \chi_{kK} \chi_{lL} \quad (3.11)$$

where  $J_{KL}$  is the microinertia tensor at the natural state of the body. With this result, it is clear that there is no need for the internal orientational directors  $\Xi_K$  in describing the macroscopic properties of the body. We only need the inertia tensor associated with a material point. Naturally, when the shape of molecular elements are known, we obtain  $J_{KL}$  in the usual way by a volume integral over the macrovolume element (or molecular element) involving internal position vectors  $\Xi_K$  within the element. For example, if we are dealing with dis-

cotic liquid crystals whose molecular elements are flat hexagonal plates, we can calculate  $J_{KL}$  of this element with respect to a set of rectangular coordinates attached to its centroid with  $\Xi_3$  pointing in the direction of the normal to the flat surface.

From (3.11), it is also clear that the symmetry properties of liquid crystals must be described by a tensor rather than a vector. In special cases, e.g. liquid crystals having rod-like molecules), one may achieve simplifications based on a vector descriptor since in such cases,  $J_{KL}$  possesses only two identical diagonal elements in the natural state. Although  $J_{KL}$  is always reducible to a diagonal matrix (generally with three non-identical entries) in a special (proper) frame, the proper frames are in general different for different molecules, so that such diagonalization is of no help in the description of the motion and in the orientational properties. Moreover, this diagonalization does not imply that the tensorial description based on  $j_{kl}$  is reducible to a vectorial description based on a director concept.

Using (2.8) in (3.11), we obtain

$$j_{kl} = G_{klmn} J_{mn}^0 \quad (3.12)$$

where

$$J_{mn}^0 = J_{MN} \delta_{mM} \delta_{nN}, \quad (3.13)$$

$$\begin{aligned} G_{klmn} = & \cos^2 \phi \delta_{km} \delta_{ln} + (\cos \phi - \cos^2 \phi)(n_k n_m \delta_{ln} + n_l n_n \delta_{km}) \\ & + (1 - \cos \phi)^2 n_k n_l n_m n_n - \sin \phi \cos \phi (\epsilon_{kmr} \delta_{ln} n_r \\ & + \epsilon_{lnr} \delta_{km} n_r) - \sin \phi (1 - \cos \phi) (\epsilon_{kmr} n_l n_n n_r \\ & + \epsilon_{lnr} n_k n_m n_r) + \sin^2 \phi \epsilon_{kmp} \epsilon_{lnr} n_p n_r. \end{aligned} \quad (3.14)$$

It is clear that  $G_{klmn}$  is a function of  $\phi_k$ , hence  $\chi_{kK}$ . Therefore, the orientational changes of the molecular elements of the body with rotatory motions are fully taken into account.

## 4 CONSTITUTIVE EQUATIONS

The state of nonlocal liquid crystals, at a point  $\mathbf{X}$  at time  $t$ , is determined by characterizing the following set of dependent variables:

$$Z = \{t_{kl}, m_{kl}, q_k, \psi, \eta, f_k, l_k, h, b\} \quad (4.1)$$

as functionals of certain independent variables that characterize the constitution of the body in motion. For the first order rate-dependent fluent bodies, the independent variables were established by us, according to the axiom of causality and objectivity (cf. 9, p. 250, 10).

$$\begin{aligned} f' &= f(\mathbf{x}') = \{\rho'^{-1}, j'_{kl}, \gamma'_{kl}, a'_{kl}, b'_{kl}, \theta', \theta'_{,k}\}, \\ g' &= g(\mathbf{x}', \mathbf{x}) = \{\mathbf{T}_{kl}, \tilde{\omega}'_k\} \end{aligned} \quad (4.2)$$

where a prime on quantities indicate that they are functions of  $x'_k$  and  $t$ ; and  $\mathbf{T}'_{kl}$  and  $\tilde{\omega}'_k$  are defined by (see 9, p. 250):

$$\mathbf{T}'_{kl} = \epsilon_{klm}(\nu'_m - \nu_m), \quad \tilde{\omega}'_k = \nu'_k - \nu_k + \frac{1}{2}(x'_l - x_l)\nu_{lk} \quad (4.3)$$

We note that all member functions listed in (4.2) are objective quantities, i.e., they transform as tensors under the time-dependent proper orthogonal transformations of the spatial coordinates. Let  $\bar{\mathbf{x}}'$  and  $\mathbf{x}'$  be two spatial frames that differ from each other by a time-dependent rigid motion, i.e.

$$\begin{aligned} \bar{\mathbf{x}}' &= \mathbf{Q}(t)\mathbf{x}' + \mathbf{b}(t), \quad \bar{\mathbf{x}} = \mathbf{Q}(t)\mathbf{x} + \mathbf{b}(t), \\ \mathbf{Q}\mathbf{Q}^T &= \mathbf{Q}^T\mathbf{Q} = \mathbf{1}, \quad \det \mathbf{Q} = 1 \end{aligned} \quad (4.4)$$

Then we have

$$\begin{aligned} \bar{f}' &= \{\rho'^{-1}, \mathbf{Q}\mathbf{j}'\mathbf{Q}^T, \mathbf{Q}\gamma'\mathbf{Q}^T \det \mathbf{Q}, \mathbf{Q}\mathbf{a}'\mathbf{Q}^T, \mathbf{Q}\mathbf{b}'\mathbf{Q}^T \det \mathbf{Q}, \theta', \mathbf{Q}\nabla\theta'\} \\ \bar{g}' &= \{\mathbf{Q}\mathbf{T}'\mathbf{Q}^T, \mathbf{Q}\tilde{\omega}'\} \end{aligned} \quad (4.5)$$

The transformation of  $f$  is identical to that of  $f'$  without primes on the tensors. The only difference between the set (4.2) and that of nonlocal micropolar fluids (9, part III, Section 9) discussed by us in the inclusion of  $\gamma'_{kl}$  to the set (4.2). For liquid crystals, this quantity is essential, since liquid crystals possess resistance to twist.

Constitutive equations of nonlocal liquid crystals may be expressed in symbolic form†

$$\mathbf{Z} = \mathcal{F}[f', g', \mathbf{r}'; f], \quad \mathbf{r}' = \mathbf{x}' - \mathbf{x} \quad (4.6)$$

which states that *each* member of (4.1) is a functional of all members of  $f', g'$ , and  $\mathbf{r}'$  and a function of  $f$ , where

$$f = f(\mathbf{x}) = \{\rho^{-1}, j_{kl}, \gamma_{kl}, a_{kl}, b_{kl}, \theta, \theta_{,k}\} \quad (4.7)$$

The response functional  $\mathcal{F}$  is scalar-valued for  $\psi, \hat{\mathbf{b}}$  and  $\hat{\mathbf{h}}$ ; vector-valued for  $\mathbf{q}, \hat{\mathbf{f}}, \hat{\mathbf{l}}$ ; and tensor-valued for  $\mathbf{t}$  and  $\mathbf{m}$ .

Constitutive functionals are subject to

- (i) The axiom of objectivity (material frame-indifference)
- (ii) The second law of thermodynamics.

† Note that  $\mathbf{x}'$  and  $\mathbf{x}$  are not objective but  $\mathbf{r}'$  is.



The axiom of objectivity requires that

$$\bar{\mathcal{F}}[f', g', r'; f] = \mathcal{F}[\bar{f}', \bar{g}', \bar{r}'; \bar{f}] \quad (4.8)$$

where

$$\bar{\mathcal{F}} = \{Q\mathbf{t}Q^T, Q\mathbf{m}Q^T \det Q, Q\mathbf{q}, \psi, \eta, Q\hat{\mathbf{f}}, Q\hat{\mathbf{l}} \det Q, \hat{h}, \hat{b}\} \quad (4.9)$$

The consequence of restrictions (4.8) is that cholesteric liquid crystals are *hemitropic*. For the nematic liquid crystals we replace (4.4)<sub>4</sub> by  $\det Q = \pm 1$  and in this case, (4.8) implies *isotropy*.†

We assume that the functions  $f', g', r'$  and  $f$  are continuously differentiable with respect to their arguments and  $f'$  and  $g'$  belong to a Hilbert space  $\mathcal{H}$  in which the inner product of two such sets of functions  $F'_1 = \{f'_1, g'_1, r'_1\}$  and  $F'_2 = \{f'_2, g'_2, r'_2\}$  are defined by

$$(F'_1, F'_2)_H = \int_{\mathbb{V}-\sigma} H(|\mathbf{x}' - \mathbf{x}|) F'_1(\mathbf{x}') \cdot F'_2(\mathbf{x}') dv(\mathbf{x}') \quad (4.10)$$

where

$$F'_1 \cdot F'_2 = f'_1 \cdot f'_2 + g'_1 \cdot g'_2 + r'_1 \cdot r'_2 \quad (4.11)$$

The influence function  $H(|\mathbf{x}' - \mathbf{x}|)$  is a positive decreasing function of  $|\mathbf{x}' - \mathbf{x}|$  such that  $H(0) = 1$ . For example, a function

$$H(|\mathbf{x}' - \mathbf{x}|) = \exp\{-\alpha|\mathbf{x}' - \mathbf{x}|\}, \quad \alpha > 0 \quad (4.12)$$

serves perfectly for this purpose. Of course, many other possibilities exist and are suggested by the atomic theory of lattices (cf. Eringen<sup>15</sup>).

The influence function is in accordance with the *attenuating neighborhood* hypothesis introduced by us.<sup>16,17</sup> It is the result of the fact that intermolecular attractions decay rapidly with distance.

The norm of  $F'$  is given by  $(F', F')_H^{1/2}$ . According to a theorem of F. Riesz, the Fréchet derivative of any functional  $\mathcal{F}(f')$  can be represented by

$$\delta\mathcal{F}(f'|\Omega) = \left( \frac{\delta\mathcal{F}}{\delta f'}, \Omega' \right)_H = \int_{\mathbb{V}-\sigma} \frac{\delta\mathcal{F}}{\delta f'}(f'; \mathbf{x}') \Omega(\mathbf{x}') dv(\mathbf{x}'), \{f', \Omega'\} \in \mathcal{H} \quad (4.13)$$

With this apparatus at hand, we can calculate the material time rate of the free energy function  $\psi$ . Thus

$$\rho\dot{\psi} = F(f', g', r'; f) \quad (4.14)$$

$$\rho\dot{\psi} = \dot{F} + Fv_{k,k} \quad (4.15)$$

† In the sense of polar fluent materials.

where we used (3.1). We have†

$$\dot{F} = \frac{\partial F}{\partial f} \dot{f} + \int_{\mathbb{V}-\sigma} \left( \frac{\delta F}{\delta f'} \dot{f}' + \frac{\delta F}{\delta g'} \dot{g}' + \frac{\delta F}{\delta r'_k} \dot{r}'_k + F v'_{k,k} \right) dv' \quad (4.16)$$

where  $dv' \equiv dv(\mathbf{x}')$ . For brevity, we introduce two operators:

$$\frac{\delta^* F}{\delta f} \equiv \frac{\partial F}{\partial f} + \int_{\mathbb{V}-\sigma} \left( \frac{\delta F'}{\delta f'} \right)^* dv' \quad (4.17)$$

$$[G\phi]_{\mathcal{A}} \equiv G\phi - (G\phi)^* \quad (4.18)$$

where an asterisk placed on parentheses indicate the interchange of  $\mathbf{x}'$  and  $\mathbf{x}$ , i.e.

$$(G(\mathbf{x}', \mathbf{x}))^* = G(\mathbf{x}, \mathbf{x}') \quad (4.19)$$

For brevity, we also introduce the following abbreviations:

$$\begin{aligned} n &= \frac{\delta^* F}{\delta \theta}, \\ {}_E t_{kl} &= -\pi \delta_{kl} - {}_E m_{kr} \gamma_{rl}, \quad {}_E m_{kl} = \frac{\delta^* F}{\delta \gamma_{lk}}, \\ {}_D t_{kl} &= t_{lk} - {}_E t_{lk}, \quad {}_D m_{kl} = m_{kl} - {}_E m_{kl}, \\ \pi &= \frac{\delta^*(F/\rho)}{\delta \rho^{-1}}, \quad F_k = \int_{\mathbb{V}-\sigma} \left[ \frac{\delta F}{\delta r'_k} - \left( \frac{\delta F}{\delta r'_k} \right)^* \right] dv', \\ \mathcal{L}_{lm} &= \frac{\partial F}{\partial j_{lr}} j_{mr} + \frac{\partial F}{\partial j_{rl}} j_{rm} + \frac{\partial F}{\partial \gamma_{lr}} \gamma_{mr} + \frac{\partial F}{\partial \gamma_{rl}} \gamma_{rm} \\ \mathcal{L}_{lm} &= \frac{\delta F}{\delta j'_{lr}} j'_{mr} + \frac{\delta F}{\delta j'_{rl}} j'_{rm} + \frac{\delta F}{\delta \gamma'_{lr}} \gamma'_{mr} + \frac{\delta F}{\delta \gamma'_{rl}} \gamma'_{rm} \end{aligned} \quad (4.20)$$

$$(4.21)$$

We now carry out various differentiations to compute  $\dot{F}$  and use (3.1), (3.2) and

$$\dot{\gamma}_{kl} = b_{kl} + v_{kr} \gamma_{rl} + v_{lr} \gamma_{kr} - \gamma_{kr} a_{lr} \quad (4.22)$$

derived in our previous work.<sup>10</sup> This gives

$$\begin{aligned} \rho \dot{\psi} &= n \dot{\theta} + {}_E t_{kl} a_{kl} + {}_E m_{kl} b_{lk} - F_k v_k \\ &\quad - \epsilon_{klm} v_k \left\{ \mathcal{L}_{lm} + \int_{\mathbb{V}-\sigma} \left[ \mathcal{L}_{lm}^* + \frac{\delta F}{\delta \tilde{\omega}'_m} (v'_l - v_l) \right] dv' \right\} \end{aligned}$$

† The last term in the integrand of (4.16) is due to the fact that  $\mathbb{V}$  is not a fixed spatial volume, but a material volume.

$$\begin{aligned}
& + \frac{\delta F}{\delta a_{kl}} \dot{a}_{kl} + \frac{\delta F}{\delta b_{kl}} \dot{b}_{kl} + \frac{\delta F}{\delta \theta_{,k}} \dot{\theta}_{',k} - \dot{v}_k \int_{\mathcal{V}-\sigma} \left[ \frac{\delta F}{\delta \tilde{\omega}'_k} - \left( \frac{\delta F}{\delta \tilde{\omega}'_k} \right)^* \right] dv' \\
& - \epsilon_{klm} \dot{v}_m \int_{\mathcal{V}-\sigma} \left[ \frac{\delta F}{\delta \Upsilon'_k} - \left( \frac{\delta F}{\delta \Upsilon'_k} \right)^* - (x'_l - x_l) \frac{\delta F}{\delta \tilde{\omega}'_k} \right] dv' - \mathcal{D} \quad (4.23)
\end{aligned}$$

with  $\mathcal{D}$  is defined by

$$\begin{aligned}
\mathcal{D} = & \int_{\mathcal{V}-\sigma} \left[ \frac{\delta F}{\delta \rho'^{-1}} \rho'^{-1} v'_{k,k} + F v'_{k,k} - \frac{\delta F}{\delta \gamma'_{kl}} \gamma'_{km} a'_{lm} + \frac{\delta F}{\delta \gamma'_{kl}} b'_{kl} + \mathcal{L}_{kl} v'_{kl} \right. \\
& + \frac{\delta F}{\delta a'_{kl}} \dot{a}'_{kl} + \frac{\delta F}{\delta b'_{kl}} \dot{b}'_{kl} + \frac{\delta F}{\delta \theta} \dot{\theta}' + \frac{\delta F}{\delta \theta'_{,k}} \dot{\theta}'_{',k} \\
& \left. + \frac{\delta F}{\delta r'_k} v'_k + \frac{\delta F}{\delta \Upsilon'_{kl}} \epsilon_{klm} \dot{v}'_m + \frac{\delta F}{\delta \tilde{\omega}'_k} \dot{v}'_k \right] dv' \quad (4.24)
\end{aligned}$$

We note that because of the antisymmetry of  $\mathcal{D}$  is  $\mathbf{x}$  and  $\mathbf{x}'$ , we have the identity

$$\int_{\mathcal{V}-\sigma} \mathcal{D} dv = 0 \quad (4.25)$$

Carrying (4.23) into (3.9), we obtain

$$\begin{aligned}
& - (\rho \eta + n) \dot{\theta} + {}_D t_{kl} a_{lk} + {}_D m_{kl} b_{lk} + \frac{1}{\theta} q_k \theta_{,k} \\
& - (\rho f_k + F_k) v_k - \left\{ \rho l_k - \rho \epsilon_{klm} x_l f_m - \epsilon_{klm} \mathcal{L}_{lm} \right. \\
& - \epsilon_{klm} \int_{\mathcal{V}-\sigma} \left[ \mathcal{L}'_{lm} + \frac{\delta F}{\delta \tilde{\omega}'_m} (v'_l - v_l) \right] dv' \left. \right\} v_k \\
& - \frac{\delta F}{\delta a_{kl}} \dot{a}_{kl} - \frac{\delta F}{\delta b_{kl}} \dot{b}_{kl} - \frac{\delta F}{\delta \theta_{,k}} \dot{\theta}'_{',k} + \dot{v}_k \int_{\mathcal{V}-\sigma} \left[ \frac{\delta F}{\delta \tilde{\omega}'_k} - \left( \frac{\delta F}{\delta \tilde{\omega}'_k} \right)^* \right] dv' \\
& + \epsilon_{klm} \dot{v}_m \int_{\mathcal{V}-\sigma} \left[ \frac{\delta F}{\delta \Upsilon'_{kl}} - \left( \frac{\delta F}{\delta \Upsilon'_{kl}} \right)^* + (x'_l - x_l) \frac{\delta F}{\delta \tilde{\omega}'_k} \right] dv' \\
& + \rho \dot{h} - \rho \theta \dot{b} - \mathcal{D} \geq 0 \quad (4.26)
\end{aligned}$$

We integrate this inequality over the volume  $\mathcal{V} - \sigma$ . This eliminates  $\rho \dot{h} - \mathcal{D}$  on account of (3.8) and (4.25). The resulting inequality is linear in the quantities  $\dot{\theta}$ ,  $v_k$ ,  $v_k$ ,  $\dot{a}_{kl}$ ,  $\dot{b}_{kl}$ ,  $\dot{v}_k$ ,  $\dot{v}_k$  and  $\dot{\theta}_{',k}$ , and therefore it cannot be maintained in one sign unless the coefficients of these quantities vanish, i.e.

$$\rho \eta = -n \quad (4.27)$$

$$\rho f_k = -F_k \quad (4.28)$$

$$\rho l_k = \epsilon_{klm} \left\{ \rho x_l f_m + \mathcal{L}_{lm} + \int_{\mathbb{V}-\sigma} \left( \mathcal{L}'_{lm} + \frac{\delta F}{\delta \tilde{\omega}'_m} (v'_l - v_l) \right) dv' \right\} \quad (4.29)$$

and

$$\begin{aligned} \frac{\delta F}{\delta a_{kl}} &= 0, \quad \frac{\delta F}{\delta b_{kl}} = 0, \quad \frac{\delta F}{\delta \theta_{,k}} = 0 \\ \int_{\mathbb{V}-\sigma} \left[ \frac{\delta F}{\delta \tilde{\omega}'_k} - \left( \frac{\delta F}{\delta \tilde{\omega}'_k} \right)^* \right] dv' &= 0 \\ \epsilon_{klm} \int_{\mathbb{V}-\sigma} \left[ \frac{\delta F}{\delta \Upsilon'_{kl}} - \left( \frac{\delta F}{\delta \Upsilon'_{kl}} \right)^* + (x'_l - x_l) \frac{\delta F}{\delta \tilde{\omega}'_k} \right] dv' &= 0 \end{aligned} \quad (4.30)$$

The entropy inequality (4.26) is now reduced to

$${}_D t_{kl} a_{lk} + {}_D m_{kl} b_{lk} + \frac{1}{\theta} q_k \theta_{,k} + \rho \dot{h} - \rho \theta \dot{b} - \mathcal{D} \geq 0 \quad (4.31)$$

To obtain implications of (4.30), it is necessary to find integrals of these equations, a task which appears to defy analytic treatment. If  $F$  is independent of  $a'_{kl}, b'_{kl}, \theta'_{,k}, \tilde{\omega}'_k, \Upsilon'_{kl}$  and  $a_{kl}, b_{kl}, \theta_{,k}$ , (4.30) is satisfied automatically. Assuming this is the case, we have

$$\rho \psi = F(\rho'^{-1}, \theta', r', \gamma'_{kl}, j'_{kl}, \rho^{-1}, \theta, \gamma_{kl}, j_{kl}) \quad (4.32)$$

$$\rho l_k = \epsilon_{klm} \left( \rho x_l f_m + \mathcal{L}_{lm} + \int_{\mathbb{V}-\sigma} \mathcal{L}'_{lm} dv' \right) \quad (4.33)$$

$$\begin{aligned} \mathcal{D} = \int_{\mathbb{V}-\sigma} \left[ \frac{\delta F}{\delta \rho'^{-1}} \rho'^{-1} v'_{k,k} + F v'_{k,k} - \frac{\delta F}{\delta \gamma'_{kl}} \gamma'_{km} a'_{lm} + \frac{\delta F}{\delta \gamma'_{kl}} b'_{lk} \right. \\ \left. + \mathcal{L}'_{kl} v'_{kl} + \frac{\delta F}{\delta \theta'} \dot{\theta}' + \frac{\delta F}{\delta r'_k} v'_k \right] dv' \end{aligned} \quad (4.34)$$

The objectivity of  $F$  and  $\mathcal{D}$  imply that the tensors

$$\begin{aligned} P_{kl} &\equiv \mathcal{L}_{kl} + \int_{\mathbb{V}-\sigma} \left( \mathcal{L}'_{kl} + \frac{\delta F}{\delta r'_k} r'_l \right) dv', \\ Q_{kl} &= \int_{\mathbb{V}-\sigma} \left[ \mathcal{L}'_{kl} + \frac{\delta F}{\delta r'_k} r'_l - \mathcal{L}'_{kl} - \left( \frac{\delta F}{\delta r'_k} r'_l \right)^* \right] dv' \end{aligned} \quad (4.35)$$

be symmetric tensors, i.e.

$$P_{kl} = P_{lk}, \quad Q_{kl} = Q_{lk} \quad (4.36)$$

From these and using (4.33), we obtain

$$\rho l_k = -\epsilon_{klm} \int_{\mathcal{V}-\sigma} \left[ \frac{\delta F}{\delta r'_k} x_l - \left( \frac{\delta F}{\delta r'_k} \right)^* x'_l \right] dv' \quad (4.37)$$

The conditions (3.8) on the residuals,  $f_k$  and  $l_k$  are now satisfied. With subsidiary conditions (4.36),  $\mathcal{D}$  is objective.

Recalling that  $\dot{\epsilon} = \dot{\psi} + \dot{\theta}\eta + \dot{\theta}\eta$ , we substitute  $\dot{\epsilon}$  into (3.5) to obtain the energy equation

$$-\rho\eta\dot{\theta} + {}_D t_{kl} a_{lk} + {}_D m_{kl} b_{lk} + q_{k,k} + \rho h + \rho \dot{h} - \mathcal{D} = 0 \quad (4.38)$$

To complete the constitutive theory, we need to write constitutive equations for  ${}_D t$ ,  ${}_D m$ ,  $q$ ,  $\dot{h}$  and  $\dot{b}$  with  $\dot{h}$  and  $\dot{b}$  subject to (3.8). In the case of no heat conduction,  $\theta$  will be uniform throughout the body, and no need arises for the energy equation (4.38). In this case, (4.31) may be integrated to give

$$\int_{\mathcal{V}-\sigma} ({}_D t_{kl} a_{lk} + {}_D m_{kl} b_{lk}) dv \geq 0 \quad (4.39)$$

From this inequality and the continuity of functionals  ${}_D t$  and  ${}_D m$  in  $\mathbf{a}$  and  $\mathbf{b}$ , it also follows that

$${}_D t = {}_D m = 0 \quad \text{when} \quad \mathbf{a} = \mathbf{b} = 0 \quad (4.40)$$

throughout  $\mathcal{V} - \sigma$ .

## 5 ADDITIVE FUNCTIONALS, QUASI-LINEAR THEORY

For a class of nonlinear functionals that are relevant to a wide class of physical problems, a representation theorem was provided by Friedman and Katz.<sup>18</sup> Let  $\mathcal{C}$  denote the class of bounded real-valued continuous functions defined in  $\mathcal{V}$ . Define the norm of a function  $f(x) \in \mathcal{C}$  by

$$||f|| = \max_{x \in \mathcal{V}} |f(x)| \quad (5.1)$$

Suppose that the functional  $F(f)$  is continuous and bounded with the norm (5.1). It is additive in the sense that for two functions,  $\{f_1, f_2\} \subset \mathcal{C}$

$$F(f_1 + f_2) = F_g(f_1) + F_g(f_2) \quad (5.2)$$

where  $F_g(f) = F(f + g) - F(g)$  for  $\{f, g\} \subset \mathcal{C}$ . Under these conditions the theorem of Friedman and Katz states that

$$F(f) = \int_{\mathcal{V}} K[f(x'), x'] dv(x') \quad (5.3)$$

We identify  $F$  with the free energy function and write

$$\rho\psi = F = \frac{\rho_0}{2} \int_{\mathbb{V}-\sigma} \Sigma(\rho'^{-1}, \theta', r'_k, \gamma'_{kl}, j'_{kl}; \rho^{-1}, \theta, \gamma_{kl}, j_{kl}) dv' \quad (5.4)$$

Since the total free energy of the body is given by

$$U = \int_{\mathbb{V}-\sigma} \rho\psi dv = \frac{\rho_0}{2} \int_{\mathbb{V}-\sigma} \int_{\mathbb{V}-\sigma} \Sigma dv' dv \quad (5.5)$$

without loss in generality, we may assume that

$$\Sigma = \Sigma^* \quad (5.6)$$

Using (5.4), and (5.6) in (4.20), (4.27) and (4.28) and (4.37), for the equilibrium parts of constitutive equations, we get

$$\eta = - \frac{\rho_0}{\rho} \int_{\mathbb{V}-\sigma} \frac{\partial \Sigma}{\partial \theta} dv' \quad (5.7)$$

$${}^E t_{kl} = -\pi \delta_{kl} - {}^E m_{kr} \gamma_{rl} \quad (5.8)$$

$$\pi = - \rho_0 \int_{\mathbb{V}-\sigma} \frac{\partial}{\partial \rho^{-1}} (\Sigma/\rho) dv' \quad (5.9)$$

$${}^E m_{kl} = \frac{\rho_0}{\rho} \int_{\mathbb{V}-\sigma} \frac{\partial \Sigma}{\partial \gamma_{lk}} dv' \quad (5.10)$$

$$f_k = - \frac{\rho_0}{\rho} \int_{\mathbb{V}-\sigma} \frac{\partial \Sigma}{\partial r'_k} dv' \quad (5.11)$$

$$l_k = - \frac{\rho_0}{\rho} \epsilon_{klm} \int_{\mathbb{V}-\sigma} \frac{\partial \Sigma}{\partial r'_k} r'_l dv' \quad (5.12)$$

For the non-equilibrium parts

$$D t_{lk} = t_{kl} - {}^E t_{kl}, \quad (5.13)$$

$$D m_{kl} = m_{kl} - {}^E m_{kl} \quad (5.14)$$

we need to write separate constitutive equations. For the incompressible materials,  $\Sigma$  is independent of  $\rho'$  and  $\rho$  and  $\pi$  is replaced by an unknown pressure function  $p$ .

With the motion, molecular elements of liquid crystals change orientations. This is affected by the change of the microinertia tensor  $j_{kl}$  and the relative directional vector  $\mathbf{r}'$  of centroids of molecules. Hence in the nonlocal theory, two types of anisotropy are present—one is due to rotations of molecules (lo-

cal and nonlocal) and the other is due to arrangements of relative locations of distant molecules with respect to the molecule at  $\mathbf{x}$ . This latter effect is a kind of "nonlocal anisotropy" which should be small as compared to the local isotropy.

The condition (5.6) implies that  $\Sigma$  depends on  $\mathbf{r}'$  through  $R'_{kl} = r'_k r'_l$ . In view of what has been said above, we replace this by  $R' = \mathbf{r}' \cdot \mathbf{r}'$  and develop a set of constitutive equations which are linear in  $\mathbf{j}$ ,  $\boldsymbol{\gamma}$ ,  $\mathbf{a}$  and  $\mathbf{b}$ . To this end, we write

$$\Sigma = \Sigma_0 + \Sigma_{ijkl} \gamma'_{ij} \gamma'_{kl} \quad (5.15)$$

where

$$\Sigma_{ijkl} = \Sigma_{ijkl}^1 + \Sigma_{ijklmn}^2 (j'_{mn} + j_{mn}) \quad (5.16)$$

Here  $\Sigma_0$ ,  $\Sigma_{ijkl}^1$  and  $\Sigma_{ijklmn}^2$  are functions of  $\rho'^{-1}$ ,  $\theta'$ ,  $R'$ ,  $\rho^{-1}$  and  $\theta$  and they are subject to the symmetry regulations

$$\begin{aligned} \Sigma_0 &= \Sigma_0^* = \Sigma_0(\rho'^{-1}, \theta', R'; \rho^{-1}, \theta), \\ \Sigma_{ijkl}^1 &= \Sigma_{ijkl}^{1*} = \Sigma_{ijkl}^1(\rho'^{-1}, \theta', R'; \rho^{-1}, \theta), \\ \Sigma_{ijklmn}^2 &= \Sigma_{ijklmn}^{2*} = \Sigma_{ijklmn}^2(\rho'^{-1}, \theta', R'; \rho^{-1}, \theta) \\ R' &= \mathbf{r}' \cdot \mathbf{r}' \end{aligned} \quad (5.17)$$

The invariance of  $\Sigma$  under rigid motions of the spatial frame of reference implies that  $\Sigma_{ijkl}^1$  and  $\Sigma_{ijklmn}^2$  are isotropic tensors, hence they can be constructed solely by means of products of  $\delta_{kl}$ . After some manipulations and using the symmetry conditions (5.17), we find that

$$\begin{aligned} \Sigma_{ijkl} &= [\Sigma_1 + \Sigma_2 \text{tr}(\mathbf{j} + \mathbf{j}')] \delta_{ij} \delta_{kl} + \Sigma_3 [(j_{ij} + j'_{ij}) \delta_{kl} \\ &\quad + (j_{kl} + j'_{kl}) \delta_{ij}] + [\Sigma_4 + \Sigma_5 (\text{tr} \mathbf{j} + \text{tr} \mathbf{j}')] \delta_{jk} \delta_{il} \\ &\quad + [\Sigma_6 + \Sigma_7 (\text{tr} \mathbf{j} + \text{tr} \mathbf{j}')] \delta_{ik} \delta_{jl} + \Sigma_8 [(j_{jk} + j'_{jk}) \delta_{il} \\ &\quad + (j_{il} + j'_{il}) \delta_{jk}] + \Sigma_9 [(j_{jl} + j'_{jl}) \delta_{ik} + \Sigma_{10} (j_{ik} + j'_{ik}) \delta_{il}] \end{aligned} \quad (5.18)$$

where

$$\Sigma_\kappa = \Sigma_\kappa^* = \Sigma_\kappa(\rho'^{-1}, \theta', R'; \rho^{-1}, \theta) \quad (5.19)$$

The equilibrium parts of constitutive equations now read:

$$\eta = -\frac{\rho_0}{\rho} \int_{\mathbf{v}-\sigma} \left( \frac{\partial \Sigma_0}{\partial \theta} + \frac{\partial \Sigma_{ijkl}}{\partial \theta} \gamma'_{ij} \gamma'_{kl} \right) d\mathbf{v}' \quad (5.20)$$

$$E^i{}_{kl} = -\pi \delta_{kl} - E m_{kr} \gamma_{rl} \quad (5.21)$$

$$\pi = -\rho_0 \int_{\mathbf{v}-\sigma} \left[ \frac{\partial(\rho^{-1} \Sigma_0)}{\partial \rho^{-1}} + \frac{\partial}{\partial \rho^{-1}} (\rho^{-1} \Sigma_{ijkl}) \gamma'_{ij} \gamma'_{kl} \right] d\mathbf{v}' \quad (5.22)$$

$$\varepsilon m_{kl} = \int_{V-\sigma} \Sigma_{ijkl} \gamma'_{ij} dv' \quad (5.23)$$

$$f_m = -2 \frac{\rho_0}{\rho} \int_{V-\sigma} \left( \frac{\partial \Sigma_0}{\partial R'} + \frac{\partial \Sigma_{ijkl}}{\partial R'} \gamma'_{ij} \gamma_{kl} \right) r'_m dv' \quad (5.24)$$

$$l_m = 0 \quad (5.25)$$

We notice that the assumption made regarding the replacement of  $\mathbf{r}'$  by  $R'$  resulted in vanishing nonlocal body couple, besides restricting the anisotropy to the orientations of molecules. In view of the fact that nonlocal gravitational couple is extremely small as compared to the couple of cohesive forces, this is certainly permissible.

It remains to construct the constitutive equations for the nonequilibrium part  ${}_D \mathbf{t}$  and  ${}_D \mathbf{m}$ . To simplify the matter, we assume that the dissipation due to rotations of molecules are negligible as compared to that due to translatory motions. This means that  $\mathbf{b}$  is not a constitutive variable. This effect has been neglected in all local theories (see our discussion in 10). The second law of thermodynamics (4.31), in this case, implies that

$${}_D \mathbf{m} = \mathbf{0} \quad (5.26)$$

The constitutive equations for  ${}_D \mathbf{t}$ , linear in  $\mathbf{j}$  and  $\mathbf{a}$ , read

$${}_D t_{ji} = \int_{V-\sigma} \alpha_{ijkl} a'_{kl} dv' \quad (5.27)$$

where

$$\begin{aligned} \alpha_{ijkl} = & \{[\alpha_1 + \alpha_2(\text{tr } \mathbf{j} + \text{tr } \mathbf{j}')] \delta_{kl} + \alpha_3(j_{kl} + j'_{kl})\} \delta_{ij} \\ & + \alpha_4(j_{ij} + j'_{ij}) \delta_{kl} + [\alpha_5 + \alpha_6(\text{tr } \mathbf{j} + \text{tr } \mathbf{j}')] \delta_{jk} \delta_{il} \\ & + [\alpha_7 + \alpha_8(\text{tr } \mathbf{j} + \text{tr } \mathbf{j}')] \delta_{ik} \delta_{jl} + \alpha_9(j_{jk} + j'_{jk}) \delta_{il} \\ & + \alpha_{10}(j_{il} + j'_{il}) \delta_{jk} + \alpha_{11}(j_{jl} + j'_{jl}) \delta_{ik} + \alpha_{12}(j_{ik} + j'_{ik}) \delta_{jl} \end{aligned} \quad (5.28)$$

If the Onsager relations are accepted, then

$$\alpha_3 = \alpha_4, \quad \alpha_9 = \alpha_{10} \quad (5.29)$$

Viscosity moduli  $\alpha_\kappa$  are subject to

$$\alpha_\kappa = \alpha_\kappa^* = \alpha_\kappa(\rho'^{-1}, \theta', R'; \rho^{-1}, \theta) \quad (5.30)$$

The axiom of objectivity is used to obtain (5.28). Of course, further restrictions to  $\alpha_\kappa$  are made by the second law of thermodynamics (4.41) so that

$$\int_{V-\sigma} \int_{V-\sigma} \alpha_{ijkl} a'_{kl} a_{ij} dv' dv \geq 0 \quad (5.31)$$



must not be violated for all possible  $\mathbf{a}$ . A set of *sufficient* conditions restricting  $\alpha_r$  were provided in our work<sup>10</sup> on local theory. These conditions may be used here too. However, investigations of the necessary and sufficient conditions for the fulfillment of (5.31) and that of non-negative free energy given by (5.5) are much more elaborate.

## 6 DIRECTOR THEORY

Molecular elements of a large class of liquid crystals are thread-like. For such liquid crystals, a great deal of simplification can be achieved by the introduction of the director concept. Suppose that  $\Xi_K$  is the common direction of the thread-like molecules at the natural state, then following our previous work,<sup>19</sup> we may write

$$\begin{aligned} d_k &= \xi_k = \chi_{kK} \Xi_K, \quad \Xi_K = \chi_{kK} d_k, \quad d_k d_k = 1 \\ \nu_{kl} &= \dot{d}_k d_l - d_k \dot{d}_l + w_{kl}, \quad \mathbf{v} = \mathbf{d} \times \dot{\mathbf{d}} + \frac{1}{2} \nabla \times \mathbf{v}, \\ a_{kl} &= d_{kl} + \dot{d}_k d_l - d_k \dot{d}_l, \quad b_{kl} = \nu_{k,l} \\ \gamma_{kl} &= \epsilon_{kmn} d_m d_{n,l}, \quad j_{kl} = I_0 (\delta_{kl} - d_k d_l) \\ \dot{\sigma}_k &= \frac{D}{Dt} (j_{kl} \nu_l). \end{aligned} \quad (6.1)$$

where  $I_0$  is the microinertia (per unit mass) of an element about an axis through the mass center, perpendicular to the long axis. As usual for the deformation tensor  $\mathbf{d}$ , vorticity tensor  $\mathbf{w}$  and the operator  $(^\circ)$ , we have

$$d_{kl} = \frac{1}{2} (\nu_{k,l} + \nu_{l,k}), \quad w_{kl} = \frac{1}{2} (\nu_{k,l} - \nu_{l,k}), \quad \dot{d}_k = \dot{d}_k - w_{kl} d_l \quad (6.2)$$

Employing (6.1) and (6.2) in the balance equations (3.1) to (3.5), and in constitutive equations (5.20) to (5.26), we obtain the basic field equations of non-local thread-like liquid crystals. The procedure is similar to our previous work on local theory.

## 7 PASSAGE TO LOCAL THEORY

When the intermolecular forces are infinitesimally short range, the material moduli  $\Sigma_r$  and  $\alpha_r$  may be considered as Dirac delta distributions, e.g.

$$\Sigma_r(R') = \Sigma_r^0 \delta(|\mathbf{x}' - \mathbf{x}|) \quad (7.1)$$

where  $\Sigma_r^0$  are functions of  $\rho'^{-1}$ ,  $\theta'$ ,  $\rho^{-1}$  and  $\theta$ . In this case, the volume integrals can be carried out reducing the constitutive equations (5.20) to (5.27), to the local forms given in our previous work<sup>10</sup> on local theory. The thermodynamic

restrictions for local theory were also studied in detail in Ref. 10. These restrictions can also be used for the nonlocal material moduli  $\Sigma_\kappa$  and viscosities  $\alpha_\kappa$ , as *sufficient conditions*. The necessary conditions requires separate investigation.

## 8 NATURE OF NONLOCAL MODULI

It is well-known that the effect intermolecular forces rapidly diminish with distance. Consequently, the material moduli  $\Sigma_\kappa$  and  $\alpha_\kappa$  must depend on  $|\mathbf{x}' - \mathbf{x}|$  or  $R'$  in such a way that as  $R'$  becomes large as compared to an internal characteristic length,  $a$ , (e.g. molecular distance, lattice parameter), the long-range effects attenuate rapidly, leading to local theory. This rough physical idea is embedded into the theory by the norm of functionals. It is known as *the axiom of attenuating neighborhood hypothesis* (Eringen<sup>16,17</sup>). This may be brought into practice by selecting the moduli  $\Sigma_\kappa$  and  $\alpha_\kappa$  in the form of functions that attenuate rapidly with  $|\mathbf{x}' - \mathbf{x}|$ . For example, we may choose

$$\Sigma_\kappa = \Sigma_\kappa^0 \exp(-\lambda R'^2/a^2) \quad (8.1)$$

where  $\Sigma_\kappa^0$  a function of  $\rho'^{-1}$ ,  $\theta'$ ,  $\rho$  and  $\theta$  and  $\lambda$  a non-dimensional adjustable parameter. Of course (8.1) must reduce to a Dirac-delta distribution in the limit  $a \rightarrow 0$  and

$$\int_{0-\infty} (\Sigma_\kappa/\Sigma_\kappa^0) dV' = 1 \quad (8.2)$$

Under these conditions in the limit as  $a \rightarrow 0$ , the nonlocal theory goes to the local theory. The situation here is similar to the case of nonlocal elasticity or fluid dynamics (cf. 3 and 20).

It may be important to remark that the adjustable parameter  $\lambda$  may be used to fit the theory with atomic lattice theories or experimental results on molecular and atomic scales.

## 9 TWO-DIMENSIONAL PROBLEMS

When the displacement and rotation fields are independent of  $x_3$ , considerable simplifications are achieved. In this case we have

$$\begin{aligned} v_1 &= v_1(x_1, x_2, t), \quad v_2 = v_2(x_1, x_2, t), \quad v_3 = 0 \\ \phi_1 &= 0, \quad \phi_2 = 0, \quad \phi_3 = \phi(x_1, x_2, t) \end{aligned} \quad (9.1)$$

The flow is in the  $(x_1, x_2)$ -plane and only rotations about  $x_3$ -axis is allowed. From (2.9) and (2.10) we have

$$\gamma_{kl} = \delta_{k3} \phi_{,l}, \quad \nu_k = \delta_{k3} \dot{\phi} \quad (9.2)$$

In order for plane flow to be possible, we must have

$$J_{13} = J_{23} = 0 \quad (9.3)$$

which is possible if the molecular elements are located in the  $(x_1, x_2)$ -plane and have vanishing thickness in  $x_3$ -direction (e.g. long axes of nematic rods are confined to  $(x_1, x_2)$ -plane). Using (3.12) to (3.14), we find that

$$\begin{aligned} j_{kl} &= J_{kl}^0 \cos^2 \phi - (\epsilon_{km3} J_{ml}^0 + \epsilon_{lm3} J_{km}^0) \sin \phi \cos \phi \\ &\quad + \epsilon_{km3} \epsilon_{ln3} J_{mn}^0 \sin^2 \phi, \quad k, l = 1, 2 \\ J_{33} &= J_{33}^0 \end{aligned} \quad (9.4)$$

Equations of motions (3.1), (3.3) and (3.5) become

$$\dot{\rho} + \rho v_{k,k} = 0 \quad (9.5)$$

$$t_{kl,k} + \rho(f_l - \dot{v}_l) + \rho \dot{f}_l = 0, \quad k, l = 1, 2 \quad (9.6)$$

$$m_{k3,k} + t_{12} - t_{21} + \rho(l_3 - j_{33} \ddot{\phi}) = 0 \quad (9.7)$$

Where the stress tensor  $t_{kl}$ , couple stress  $m_{k3}$  and the body force residual  $f_l$  are obtained by using (4.20), (5.21) to (5.24), (5.18), (5.28), (9.2) and (9.3). Hence

$$t_{kl} = {}_E t_{kl} + {}_D t_{lk} \quad (9.8)$$

$$m_{k3} = {}_E m_{k3} = \int_{\mathcal{A}-\sigma} [\sigma_0 \delta_{kl} + \sigma_1 (j_{kl} + j'_{kl})] \phi'_{,l} da' \quad (9.9)$$

$${}_E t_{kl} = -\pi \delta_{kl} - m_{k3} \phi_{,l} \quad (9.10)$$

$${}_D t_{kl} = \int_{\mathcal{A}-\sigma} \alpha_{lkij} a'_{ij} da' \quad (9.11)$$

where  $\alpha_{kl ij}$  is given by (5.28) and

$$\sigma_0 = \Sigma_6 + \Sigma_7(\text{tr } \mathbf{j} + \text{tr } \mathbf{j}') + \Sigma_{10}(j_{33} + j'_{33}), \quad (9.12)$$

$$\sigma_1 = \Sigma_9$$

All indices have the range (1,2). Within the realm of the linear constitutive theory  $\pi$  and  $f_k$  are given by

$$\pi = -\rho_0 \int_{\mathcal{A}-\sigma} \frac{\partial}{\partial \rho^{-1}} (\rho^{-1} \Sigma_0) da', \quad (9.13)$$

$$f = -2 \frac{\rho_0}{\rho} \int_{\mathcal{A}-\sigma} \frac{\partial \Sigma_0}{\partial R'} (\mathbf{x}' - \mathbf{x}) da' \quad (9.14)$$

In the context of the two-dimensional theory we also have two-dimensional non-locality which requires that the volume integrations over  $\mathcal{V} - \sigma$  is replaced by integrations over the  $(x_1, x_2)$ -plane  $(\mathcal{A} - \sigma)$ .

The field equations for  $\rho$ ,  $\mathbf{v}$  and  $\phi$  follow from (9.5) to (9.7) and (9.8) to (9.11)

$$\rho + \rho v_{k,k} = 0, \quad (9.15)$$

$$-\pi_{,l} - \frac{\partial}{\partial x_k} \int_{\Omega-\sigma} \{[\sigma_0 \phi'_{,k} + \sigma_1(j_{km} + j'_{km}) \phi'_{,m}] \phi_{,l} - \alpha_{klj} a'_{ij}\} da' \\ + \rho(f_l - \dot{v}_l) + \rho f_l = 0 \quad (9.16)$$

$$\frac{\partial}{\partial x_k} \int_{\Omega-\sigma} [\sigma_0 \phi'_{,k} + \sigma_1(j_{kl} + j'_{kl}) \phi'_{,l}] da' + \int_{\Omega-\sigma} [\sigma_0(\phi'_{,2} \phi_{,1} - \phi'_{,1} \phi_{,2}) \\ + \sigma_1(j_{2l} + j'_{2l}) \phi'_{,l} \phi_{,1} - \sigma_1(j_{1l} + j'_{1l}) \phi'_{,l} \phi_{,2} \\ + (\alpha_{12ij} - \alpha_{21ij}) a'_{ij}] da' + \rho(l_3 - j_{33} \ddot{\phi}) = 0 \quad (9.17)$$

where

$$a'_{ij} = v'_{i,j} - \epsilon_{ij3} \dot{\phi}' \quad (9.18)$$

Given the state function  $\Sigma_0$  the set (9.15) to (9.17) constitutes four integro-partial differential equations for determination of four unknown functions  $\rho$ ,  $v_k$  and  $\phi$ .

### A Steady, plane shear flows

For steady plane shear flows, we have

$$v_1 = v(y), \quad v_2 = v_3 = 0, \quad \phi_3 = \phi(y)$$

where we set  $x_2 = y$ . Consequently

$$\gamma_{kl} = \delta_{k3} \delta_{l2} \frac{d\phi}{dy}, \quad a_{kl} = \frac{dv}{dy} \delta_{k2} \delta_{l1} \quad (9.20)$$

For incompressible fluids, we replace  $\pi$  with an unknown pressure  $p(x, t)$ . If body forces and couples are absent, then (9.16) and (9.17) simplify to:

$$-p_{,l} - \frac{\partial}{\partial y} \int_{-\infty}^{\infty} \{[\sigma_0 + \sigma_1(j_{22} + j'_{22}) \phi'_{,2} \phi_{,2} \delta_{l2} - \alpha_{2l21} v'_{,2}]\} dy', \quad (9.21)$$

$$\frac{\partial}{\partial y} \int_{-\infty}^{\infty} [\sigma_0 + \sigma_1(j_{22} + j'_{22})] \phi'_{,2} dy' + \int_{-\infty}^{\infty} [-\sigma_1(j_{12} + j'_{12}) \phi'_{,2} \phi_{,2} \\ + (\alpha_{1221} - \alpha_{2121}) v'_{,2}] dy' = 0 \quad (9.22)$$

For  $l = 2$  (9.21) is integrated to give the pressure

$$p(x, y) = p_0(x) - \int_{-\infty}^{\infty} \{[\sigma_0 + \sigma_1(j_{22} + j'_{22}) \phi'_{,2} \phi_{,2} - \alpha_{2221} v'_{,2}]\} dy' \quad (9.23)$$

and for  $l = 1$  it gives

$$\int_{-\infty}^{\infty} \alpha_{2121} v'_{,2} dy' = p_{0,x} y + C_1 \quad (9.24)$$

where  $p_0(x)$  and  $C_1$  are integration function and constant, respectively. Equations (9.22) and (9.24) are two integro-partial differential equations for the determination of  $v$  and  $\phi$ .

In the case of thread-like elements selecting the same rectangular frame of reference for both material and spatial coordinates, we have

$$J_{11}^0 = 0, \quad J_{22}^0 = J_{33}^0 = J_0, \quad J_{12}^0 = J_{13}^0 = J_{23}^0 = 0 \quad (9.25)$$

and (9.4) gives

$$j_{11} = J_0 \sin^2 \phi, \quad j_{22} = J_0 \cos^2 \phi, \quad j_{12} = -J_0 \sin \phi \cos \phi \quad (9.26)$$

where  $\phi$  is now the angle between the long axis of threads and the  $x$ -axis. Using (9.26), (9.23), (9.24), and (9.22) may be expressed as:

$$p(x, y) = p_0(x) - \int_{-\infty}^{\infty} \{[s_0 + s_1(\cos 2\phi + \cos 2\phi')] \phi'_{,2} \phi_{,2} + \lambda_0(\sin 2\phi + \sin 2\phi') v'_{,2}\} dy', \quad (9.27)$$

$$\int_{-\infty}^{\infty} [\lambda_1 - \lambda_2(\cos 2\phi + \cos 2\phi')] v'_{,2} dy' = p_{0,x} y + C_1, \quad (9.28)$$

$$\frac{d}{dy} \int_{-\infty}^{\infty} [s_0 + s_1(\cos 2\phi + \cos 2\phi')] \phi'_{,2} dy' + \int_{-\infty}^{\infty} [s_1(\sin 2\phi + \sin 2\phi') \phi'_{,2} \phi_{,2} + \lambda v'_{,2}] dy' - p_{0,x} y - C_1 = 0, \quad (9.29)$$

where

$$\begin{aligned} s_0 &= \sigma_0 + \sigma_1 J_0 = \Sigma_6 + J_0(4\Sigma_7 + \Sigma_9 + 2\Sigma_{10}), \\ s_1 &= \frac{1}{2} \sigma_1 J_0 = \frac{1}{2} J_0 \Sigma_9 \\ \lambda_0 &= \frac{1}{2} J_0(\alpha_3 + \alpha_{10} + \alpha_{11}), \\ \lambda_1 &= \alpha_7 + J_0(4\alpha_8 + \alpha_{11} + \alpha_{12}), \\ \lambda_2 &= \frac{1}{2} (a_{11} - \alpha_{12}) J_0, \\ \lambda &= \alpha_5 + J_0(4\alpha_6 + 2\alpha_9) \end{aligned} \quad (9.30)$$

are functions of  $|y' - y|$ .

## B Twist waves

Here we consider propagations of twist waves in an *ideal* liquid crystal (in-

compressible and inviscid) occupying  $(x, y)$ -plane. The rotation angle  $\phi$  is assumed to be small and the velocity  $\mathbf{v} = \mathbf{0}$ . Suppose that a plane torsional disturbance is imparted to the body propagating in  $y$ -direction. For instance, such a disturbance can emanate from a vibrating wall at  $y = 0$  to the liquid crystal occupying the region  $y > 0$ . The effective nonlocality is in the  $y$ -direction.

We have  $\alpha_{klij} = 0$ ,  $\mathbf{f} = \hat{\mathbf{f}} = \mathbf{l} = \mathbf{0}$  and

$$\mathbf{v} = \mathbf{0}, \quad \phi = \phi(y) \quad (9.31)$$

Equation (9.16) is integrated to determine the unknown pressure  $\pi = p$ , i.e.

$$p = p_0 + \int_{-\infty}^{\infty} [\sigma_0 \phi'_{,2} + \sigma_1 (j_{22} + j'_{22}) \phi'_{,2}] \phi_{,2} dy' \quad (9.32)$$

Equation (9.17) is linearized to read

$$\frac{\partial}{\partial y} \int_{-\infty}^{\infty} \sigma(|y - y'|) \frac{\partial \phi}{\partial y'} dy' - \rho J_0 \frac{\partial^2 \phi}{\partial t^2} = 0 \quad (9.33)$$

where

$$\sigma(|y - y'|) = \sigma_0 + 2\sigma_1 J_0 \quad (9.34)$$

In the linearization of (9.17), we used (9.26) for the microinertia, which is valid for liquid crystals having thread-like elements.

For one-dimensional non-locality, the following exponential kernel is known to approximate intermolecular attenuation adequately.

$$\sigma = \mu_0 \frac{k}{2} \exp(-k|y - y'|) \quad (9.35)$$

where  $\mu_0$  is a material constant. We note that this kernel is a delta-sequence and it satisfies

$$\int_{-\infty}^{\infty} \sigma dy' = \mu_0 \quad (9.36)$$

Equation (9.33) now reads

$$\frac{\partial}{\partial y} \int_{-\infty}^{\infty} \mu_0 \frac{k}{2} e^{-|y-y'|} \frac{\partial \phi}{\partial y'} dy' - \rho J_0 \frac{\partial^2 \phi}{\partial t^2} = 0 \quad (9.37)$$

By differentiating (9.37) twice, with respect to  $y$ , we obtain:

$$\frac{\partial^4 \phi}{\partial y^2 \partial t^2} - k^2 \frac{\partial^2 \phi}{\partial t^2} + \frac{\mu_0 k^2}{\rho J_0} \frac{\partial^2 \phi}{\partial y^2} = 0 \quad (9.38)$$

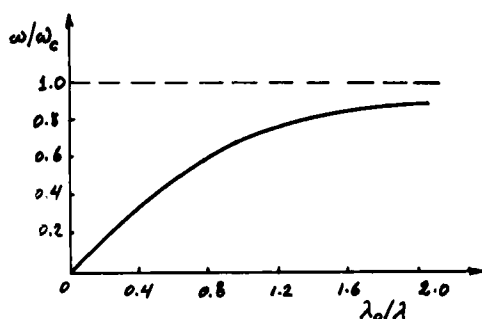


FIGURE 1 Dispersion curve.  
 $\lambda_0 \equiv c_0 2\pi/\omega_c$

A plane-wave solution of this equation is given by

$$\phi = \phi_0 \exp \left[ i \left( \frac{2\pi}{\lambda} y + \omega t \right) \right] \quad (9.39)$$

where the wave length  $\lambda$  is determined by

$$\frac{\lambda}{2\pi} = c_0 [1 - (\omega/\omega_c)^2]^{1/2} \omega^{-1} \quad (9.40)$$

with

$$\omega_c = (\mu_0/\rho J_0)^{1/2} k \quad (9.41)$$

From (9.40), it is clear that the *twist-waves are dispersive*. Moreover, they possess a *cut-off* frequency which is  $\omega = \omega_c$ . The dispersion curve is sketched in Figure 1. The phase velocity  $c$  is given by

$$c = c_0 [1 - (\omega/\omega_c)^2]^{3/2}, \quad \omega \leq \omega_c \quad (9.41)$$

Where  $c_0 = (\mu_0/\rho J_0)^{1/2}$  is the phase velocity at the origin (infinite wave length).

It is interesting to note that if the nonlocality is absent (i.e. in the local theory), (9.37) takes the form

$$\mu_0 \frac{\partial^2 \phi}{\partial y^2} - \rho J_0 \frac{\partial^2 \phi}{\partial t^2} = 0 \quad (9.43)$$

which leads to non-dispersive twist waves with constant phase velocity  $c_0$ . The dispersive nature of twist waves are well-known from experiments and solid state considerations.

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