

**LIQUID CRYSTALS WITH VARIABLE
DEGREE OF ORIENTATION**

By

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1. Introduction. For the small-molecule nematic liquid crystals commonly used in display devices, what Chandrasekhar [1] calls the Oseen-Zöcher-Frank equations, hereafter referred to as the OZF equations, have been quite successful in describing many static phenomena. For phenomena involving flow, what he calls the Ericksen-Leslie equations have been used rather successfully: they reduce to the OZF equations, for statics. Many workers accept what he calls Parodi's relation, an Onsager relation. Careful experimental tests of this have not been made, as far as I know. Currie [2] points out that it does have some status, as a stability condition. Kuzuu and Doi [3] note that the type of molecular theory which they consider does imply this relation. I follow de Gennes [4] in referring to the resulting equations as the EL or ELP theory, depending on whether Parodi's relation is presumed to hold.

Two things have motivated me to consider modifying the equations. For one thing, I am interested in seeing the development of a mathematically sound theory of defects which might be at rest, or moving. The static theory of point defects, based on the OZF equations, is now rather well developed, as is discussed in surveys by Ericksen [5] and Kinderlehrer [6]. I believe that the EL and ELP theories are capable of describing moving point defects. However, no real progress has been made in developing pertinent analyses, despite some serious efforts. More serious difficulties are encountered with some observed kinds of disclinations (line defects). According to the aforementioned theories, these more violent singularities cause energy integrals, *etc.* to diverge. In dealing with rather specific situations, workers have patched up the theory, by excluding a tube of small radius, assigning a finite "core energy" to it. I just don't believe that one can use such ideas as a basis for developing satisfactory mathematical theory, particularly for moving defects. Such phenomena are of interest for both nematic and cholesteric liquid crystals. In the latter, they are associated with the interesting "blue phases" discussed by Cladis [7] and Sethna [8], among other things.

In tinkering with theories which work rather well, there is some danger that, in fixing one flaw, one will find other good predictions affected adversely. Slowly, I have come to the view that the risk is worth taking. There is a physically reasonable way of modifying the equations to help tame the singularities, discussed a bit for static problems by Fan [9], some years ago. Essentially, I will elaborate and generalize this. Roughly, it involves introducing an additional scalar variable, the so-called degree of orientation. With this comes a kind of elasticity not represented in the EL theory. As is to be discussed, this and another mechanism are involved in various molecular theories of liquid crystal polymers which are more or less like that of Doi [11]. The format presented by Macmillan [11] is

flexible enough to cover most proposals of this kind. So, the theory to be discussed can be viewed as a kind of compromise between the EL or ELP theories, and theories of the latter kind. Observations of such polymers do seem to indicate much more complex behavior than is common for the small molecule liquid crystals. There is then plenty of room for differences of opinion as to how best to develop theory for them.

Some good analysts have helped me to get some feeling for the modified theory, by studying special forms of the equations or some which are at least very similar. Informally, they have also helped me by showing educated guesses as to what might be provable. Concerning the defects, work by Hardt [12], Lin [13] and Maddocks [14] have reinforced my impression that the modified theory provides a decent basis for developing a sound theory of line defects, and that it might be feasible to do so. Lin, particularly, helped me to see a possibility, which had not before entered my mind, that the seemingly more complicated equations might, in fact, be more tractable, for dealing with the problems of moving point defects, than the EL equations. I won't claim that this is an established fact, but do believe that it is a good possibility. In the liquid crystal polymers, observations seem to indicate that it is rather common for defects to occur in large numbers, perhaps including surface defects, associated with the "domain" structures such as are mentioned by Wissbrun [15], for example. I am not so sanguine about finding good ways of dealing with the large numbers, but it might be feasible to determine whether equations of the kind considered permit solutions of the surface-defect kind. Concerning the polymers, Calderer [16,17,18] has done some interesting analyses, using special forms of the equations, relating to flow phenomena observed in such liquids.

There is some prejudice that the EL equations represent asymptotic approximations to various more general equations included in MacMillan's [11] format, for very slow flows. He gives the best available analysis of this, which is rigorous, but applicable only to a very special set of situations. It has become clear that tricky singular perturbation theory is involved, as was first realized by Kuzuu and Doi [3], as far as I know. One could try some analogous asymptotic analysis, allowing for defects. However, this is too tricky for me and, I expect, would be possible only subject to judicious assumptions about unknown constitutive equations. In working through the program, we will, in part, get some assessment of likely assumptions. I have written as if I accepted the notion that theories included in MacMillan's [11] format are clearly the most sound. There is room to argue about this, and he does discuss some of the pros and cons. I do find it interesting that the bulk of the experimentation on polymers seems to fit the present format as comfortably as it does the more complex format indicated. In this respect, the coverage by Wissbrun [15] is, I think, reasonably representative. So, it seems that this intermediate theory could be rather useful, as a basis for understanding some phenomena relating to the polymers, Calderer's [16,17,18] work being a first step in this direction.

2. Orientation Variables. Much of the interest in liquid crystals is associated with efforts to control their orientation, so relevant theory needs to introduce variable(s) to

describe this, in the situations likely to be of most interest. Among those concerned with relevant molecular theory, there is some consensus of opinion that a good choice is a second-order tensor \mathbf{M} , representing a second order moment of an (unknown) orientation distribution function associated with the rather rigid, more or less rod-like molecules. There is some debate about this but, without further ado, I accept it. Experimental estimates of it involve assuming that it is simply related to something else which is more accessible experimentally, often the dielectric tensor associated with optical observations. From its definition, it has some properties which do not depend on the form of the distribution function, *viz.*

$$(2.1) \quad \mathbf{M} = \mathbf{M}^T, \text{tr} \mathbf{M} = 1, \mathbf{M} \geq 0$$

the latter inequality meaning that the eigenvalues of \mathbf{M} are non-negative. Actually, they are positive unless the directions of the little rods are all either parallel or perpendicular to the same direction. My prejudice is that such configurations are unattainable, physically. As a personal matter, I don't feel very comfortable with equations of motion or equilibrium for \mathbf{M} which permit values to violate (2.1).

Following common practice, we use instead of \mathbf{M} its deviator

$$(2.2) \quad \mathbf{Q} = \mathbf{M} - 1/3,$$

with eigenvalues $Q_n (n = 1, 2, 3)$ satisfying

$$(2.3) \quad \begin{cases} -1 \leq 3Q_n \leq 2, Q_1 + Q_2 + Q_3 = 0, \\ -2 \leq 3(Q_1 + Q_2) \leq 1, \text{etc.} \end{cases}$$

In the sense made clear by this, \mathbf{Q} is a fairly small tensor and it is rather common to assume that various functions of interest can be approximated well enough by polynomials of rather low degree in \mathbf{Q} . We will consider this, partly because we need the first few terms in expansions about $\mathbf{Q} = 0$, for a different reason.

In terms of \mathbf{Q} , we can distinguish three kinds of configurations. One consists of the randomly oriented or *isotropic* configurations, with

$$(2.4) \quad \mathbf{Q} = 0,$$

the only configurations for which $Q_1 = Q_2 = Q_3$. Then, there are the *nematic* configurations, for which exactly two of the three eigenvalues coincide. Then \mathbf{Q} can be and commonly is represented in the form

$$(2.5) \quad \mathbf{Q} = S(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{1}), \mathbf{n} \cdot \mathbf{n} = 1, -1/2 \leq S \leq 1,$$

where the scalar S is called the *degree of orientation*. By a reasonable interpretation the OZF, EL and ELP theories presume that (2.5) always applies, with S a function of the temperature θ only. Then, the eigenvector \mathbf{n} , called the *director* is commonly identified with the optic axis of these optically uniaxial liquids. Of course, this is one way to keep values of \mathbf{Q} in the physically meaningful domain. The names are a bit confusing in that (2.5) is also considered to apply to what many call cholesteric liquid crystals. The important difference is one of material symmetry. Nematics display symmetry with respect to reflections, while the cholesterics don't: their molecules have a symmetry more like that of a helical spring than that of a rod. Some refer to cholesterics as chiral nematics, which is more apt. In either of these kind of nematic liquids, what workers commonly mean by defects are points or curves where the optic axis is undefined. Mathematically, \mathbf{n} would be ill-defined at, say, isolated points where S vanishes. As noted above, the OZF and EL theories won't let S vanish. Roughly, Fan's [9] idea is to modify the theory so that S can vanish at defects, where \mathbf{n} is undefined. He noted some evidence that this can tame the singularities enough to let integrals of interest converge. For reasonable governing equations, one then needs to prove theorems concerning the sets on which S can vanish, how this compares to sets on which \mathbf{n} is singular *etc.*. As is discussed by Hardt [12] and Lin [13], some good theorems of this kind have been proved. So, there is some reason to believe that it is feasible to begin to develop a mathematically sound theory of defects, by following his line of thought.

There is the third possibility, that the three eigenvalues of \mathbf{Q} are all distinct, giving what are called *biaxial nematic* configurations. Theories fitting MacMillan's [11] format permit any of the three types of configurations to occur. Certainly it is not unreasonable to think that flows or other influences could convert a rather stable nematic configuration to one of the biaxial type, *etc.*. I [19] am one of those who have argued that, near isotropic-nematic phase transitions, it should be quite easy to induce such changes. Accounting for such possibilities does add significant complications to the equations, and the problems of analyzing them. Experimental information concerning the biaxial configurations is still quite slim and, for me, it is too early to think seriously about them. So, I will develop theory representing a kind of compromise. Basically, it generalizes the EL or ELP theories, by introducing the scalar S as a variable. Concerning constitutive equations, I will insist upon some consistency with those used in the theories permitting the biaxial configurations. Necessarily, the equations of motion will be rather different. So, the only real difference concerns allowing for such a splitting of eigenvalues, if we are concerned with what are normal stable nematic phases, in equilibrium. The theories of the kinds mentioned are all of the near equilibrium kind, it being a matter of guesswork as to how far we can push them, before getting into serious trouble.

Formally, theory to be discussed is quite similar to theories involving a vector field with variable magnitude, such as is discussed by Leslie [20], for example. Hardt [12] and Lin [13] treat some special cases which do fit this mold. In general, it is at least tricky

to get a good mesh between these two kinds of theory. The idea is try to introduce some vector \mathbf{m} , depending on S and \mathbf{n} , which adequately describes both S and \mathbf{n} . Physically, \mathbf{n} is equivalent to $-\mathbf{n}$, but S and $-S$ describe physically different configurations. With the vector description, it seems hard to incorporate these distinctions. For example, we could write

$$(2.6) \quad \begin{cases} \mathbf{Q} &= \mathbf{m} \otimes \mathbf{m} - \frac{1}{3}|\mathbf{m}|^2 \mathbf{1}, \mathbf{m} = \sqrt{S}\mathbf{n}, \text{ when } S \geq 0, \\ &= -\mathbf{m} \otimes \mathbf{m} + \frac{1}{3}|\mathbf{m}|^2 \mathbf{1}, \mathbf{m} = \sqrt{-S}\mathbf{n}, \text{ when } S \leq 0, \end{cases}$$

formally relating \mathbf{Q} to a vector. Given \mathbf{m} , we then don't get a unique value of \mathbf{Q} unless we independently fix the sign of S , and there is no obvious way to determine this, given only the value of \mathbf{m} . From considerations of this kind, I conclude that the two kinds of theories are really different, although one might well borrow or adapt ideas and analyses from one to develop the other.

3. Basic Format. Here, I briefly sketch the format used to generate equations for the quantities of interest, taken to be the fields S and \mathbf{n} , the velocity \mathbf{v} and the absolute temperature θ . As might be expected from the preceding discussion, the considerations are not very different from those used by Leslie [20] and they also fit pretty well the general format discussed by Ericksen [21], so I will try to be brief. Here, the fields and constitutive equations are considered as smooth.

I accept the usual idealization of these liquids as incompressible materials, with constant mass density ρ and \mathbf{v} satisfying the usual equation of continuity

$$(3.1) \quad \nabla \cdot \mathbf{v} = 0.$$

Also, from $(2.5)_2$, the director is to satisfy the constraint

$$(3.2) \quad \mathbf{n} \cdot \mathbf{n} = 1.$$

For \mathbf{v} , I use the customary balance of linear momentum. In integral form, we have

$$(3.3) \quad \frac{d}{dt} \int_{\Omega} \rho \mathbf{v} d\mathbf{x} = \int_{\partial\Omega} \boldsymbol{\sigma} d\mathbf{x} + \int_{\Omega} \mathbf{f} d\mathbf{x},$$

with Ω an arbitrary material region, or the differential equivalent

$$(3.4) \quad \rho \dot{\mathbf{v}} = \nabla \cdot \boldsymbol{\sigma} + \mathbf{f},$$

where the superposed dot denotes the material derivative. Here, $\boldsymbol{\sigma}$ is the (asymmetric) stress tensor, \mathbf{f} the body force per unit volume.

For S and \mathbf{n} , I use rather similar formats. For S , it is a scalar equation of the form

$$(3.5) \quad \dot{P} = \nabla \cdot \mathbf{T} + G^I + G^E.$$

Here, P represents a generalized momentum, with the terms on the right representing generalized forces. Briefly, G^I represents a kind of internal body force, G^E being associated with external effects, like applied electromagnetic fields. Similarly, for \mathbf{n} , we have a vector equation of the form

$$(3.6) \quad \dot{\pi} = \nabla \cdot \tau + \mathbf{g}^I + \mathbf{g}^E,$$

interpreted in an analogous way. Roughly, there are the “forces of constraint”, associated with (3.1) and (3.2), entirely similar to those considered by Leslie [20], in his treatment of the EL theory. For θ , we start with an energy balance of the form

$$(3.7) \quad \begin{aligned} \frac{d}{dt} \int_{\Omega} (e + \frac{1}{2} \rho |\mathbf{v}|^2) d\mathbf{x} &= \int_{\partial\Omega} [(\mathbf{v} \cdot \boldsymbol{\sigma} + \dot{\mathbf{n}} \cdot \boldsymbol{\tau}) d\mathbf{S} + (\dot{S} \mathbf{T} - \mathbf{q}) \cdot d\mathbf{S}] \\ &+ \int_{\Omega} (\mathbf{f} \cdot \mathbf{v} + G^E \dot{S} + \mathbf{g}^E \cdot \mathbf{n} - r) d\mathbf{x}. \end{aligned}$$

On the left, we have separated out the obvious translational kinetic energy, but e can include rotational kinetic energy associated with motion of \mathbf{n} , for example. Also, \mathbf{q} is the heat flux vector, r covering rate of heating in the interior. Going to the differential equivalent, and using the preceding equations to rearrange this, we get

$$(3.8) \quad \begin{aligned} \dot{e} &= \text{tr}[\nabla \mathbf{v} \boldsymbol{\sigma}^T + \nabla(\dot{\mathbf{n}}) \boldsymbol{\tau}^T] + \nabla \dot{S} \cdot \mathbf{T} \\ &+ (\dot{P} - G^I) \dot{S} + (\dot{\pi} - \mathbf{g}^I) \cdot \dot{\mathbf{n}} - \nabla \cdot \mathbf{q} - r. \end{aligned}$$

As a form of the second law, I accept the Clausius-Duhem inequality,

$$(3.9) \quad \dot{\eta} \geq \nabla \cdot (\mathbf{q}/\theta) + r/\theta,$$

where η is the entropy per unit volume. Leslie [20] considers a more general form, which leads to some differences in conclusions. In my opinion, the differences are of minor import, physically, and at least for the present, it seems to me better to exclude these complications. We now introduce

$$(3.10) \quad \varphi = e - P \dot{S} - \dot{\pi} \cdot \dot{\mathbf{n}} - \theta \eta,$$

which I'll call the Helmholtz free energy density, although it also resembles action. By using this, and eliminating $\nabla \cdot \mathbf{q} + r$ between (3.8) and (3.9), one gets the inequality

$$(3.13) \quad \begin{aligned} \dot{\varphi} &\leq \text{tr}[\nabla \dot{\mathbf{v}}(\boldsymbol{\sigma}^T + \boldsymbol{\tau}^T \nabla \mathbf{n} + \mathbf{T} \otimes \nabla \mathbf{S})] \\ &- P \ddot{S} - G^I \dot{S} + \overline{\nabla S} \cdot \mathbf{T} - \dot{\pi} \cdot \ddot{\mathbf{n}} - \mathbf{g}^I \cdot \dot{\mathbf{n}} \\ &+ \text{tr}(\overline{\nabla \mathbf{n}} \boldsymbol{\tau}^T) - \mathbf{q} \cdot \nabla \theta / \theta. \end{aligned}$$

As usual, the idea is to use this to get restrictions on constitutive equations, here for $\varphi, \sigma, P, \mathbf{T}, G^I, \dot{\pi}, \mathbf{g}^I$ and \mathbf{q} . Following the pattern of theories mentioned earlier, I assume that, except for terms of the Lagrangian multiplier kind, associated with the constraints, these are functions of the list

$$(3.14) \quad \mathbf{n}, \dot{\mathbf{n}}, \nabla \mathbf{n}, S, \dot{S}, \nabla S, \nabla \mathbf{v}, \theta, \nabla \theta.$$

Then, by arguments much like those used by Leslie [20], one can deduce that

$$(3.15) \quad \left\{ \begin{array}{l} \varphi \text{ is in dependent of } \nabla \mathbf{v} \text{ and } \nabla \theta, \\ \sigma = -p1 - \nabla \mathbf{n}^T \frac{\partial \varphi}{\partial \nabla \mathbf{n}} - \nabla S \otimes \frac{\partial \varphi}{\partial \nabla S} + \hat{\sigma}, \\ P = -\frac{\partial \varphi}{\partial \dot{S}}, \\ T = \frac{\partial \varphi}{\partial \nabla S}, \\ G^I = -\frac{\partial \varphi}{\partial \dot{S}} + \hat{G}, \\ \pi = -\frac{\partial \varphi}{\partial \dot{\mathbf{n}}} + a\mathbf{n}, \\ \tau = \frac{\partial \varphi}{\partial \nabla \mathbf{n}} + \mathbf{n} \otimes \mathbf{b}, \\ \mathbf{g}^I = -\frac{\partial \varphi}{\partial \dot{\mathbf{n}}} + a\dot{\mathbf{n}} - \nabla \mathbf{n} \mathbf{b} + c\mathbf{n} + \hat{\mathbf{g}}, \\ \eta = -\frac{\partial \varphi}{\partial \theta}, \end{array} \right.$$

(3.13) then reducing to

$$(3.16) \quad \Delta \stackrel{def}{=} tr(\nabla \mathbf{v} \hat{\sigma}^T) - \hat{\mathbf{g}} \cdot \dot{\mathbf{n}} - \hat{G} \dot{S} - \mathbf{q} \cdot \nabla \theta / \theta \geq 0,$$

with Δ as a measure of dissipation. In (3.15), p is the usual arbitrary pressure, a Lagrange multiplier associated with (3.1). Similarly, the scalars a and c and vector \mathbf{b} are arbitrary functions of position and time, multipliers associated with (3.2).

There are the various implications of invariance, again much like those discussed by Leslie [20]. In part, most of the constitutive equations are assumed to be invariant under the group of smooth rigid motions or, briefly, to be objective. There is one caveat, in that the assumption is not so reasonable for φ , which might cover rotational kinetic energy. For it, it is reasonable to assume that it is at least invariant under Galilean transformations, involving the time-independent rotations and translations depending linearly on time. Then, by reasoning which is essentially the same as that used by Ericksen [22], one gets the differential identity

$$(3.17) \quad \mathbf{U} \stackrel{def}{=} \mathbf{n} \otimes \frac{\partial \varphi}{\partial \mathbf{n}} + \dot{\mathbf{n}} \otimes \frac{\partial \varphi}{\partial \dot{\mathbf{n}}} + \nabla \mathbf{n}^T \frac{\partial \varphi}{\partial \nabla \mathbf{n}} - \frac{\partial \varphi}{\partial \nabla \mathbf{n}} \nabla \mathbf{n}^T \equiv \mathbf{U}^T.$$

Similarly, the parts of σ , *etc.* depending explicitly on φ might well only exhibit this lesser invariance, but I think it reasonable to assume that remainders, like $\hat{\sigma}, \hat{G}$ *etc.* are objective,

and that this also applies to Δ . This produces a differential identity, formally identical to that used in the EL theory.

$$(3.18) \quad \hat{\sigma} - \hat{\sigma}^T = \hat{\mathbf{g}} \otimes \mathbf{n} - \mathbf{n} \otimes \hat{\mathbf{g}}.$$

This, along with (3.15) and (3.17) produces another identity

$$(3.19) \quad \sigma - \sigma^T = \nabla \mathbf{n} \tau^T - \tau \nabla \mathbf{n}^T + \mathbf{g}^I \otimes \mathbf{n} - \mathbf{n} \otimes \mathbf{g}^I + \pi \otimes \dot{\mathbf{n}} - \dot{\mathbf{n}} \otimes \pi,$$

as a replacement of Cauchy's condition that the stress tensor be symmetric. As in the EL theory, this produces a balance law implied by previous equations for \mathbf{v} *etc.*,

$$(3.20) \quad \begin{aligned} \frac{d}{dt} \int_{\Omega} (\mathbf{x} \wedge \rho \mathbf{v} + \mathbf{n} \wedge \pi) d\mathbf{x} &= \int_{\partial\Omega} (\mathbf{x} \wedge \sigma d\mathbf{S} + \mathbf{n} \wedge \tau d\mathbf{S}) \\ &+ \int_{\Omega} (\mathbf{x} \wedge \mathbf{f} + \mathbf{n} \wedge \mathbf{g}^E) d\mathbf{x}. \end{aligned}$$

As is discussed by Stephen and Straley [23], one can view (3.6) as the equation guaranteeing the balance of couples involved in (3.20). This has helped to identify some of the pieces, physically: $\mathbf{n} \wedge \mathbf{g}^E$ is a body couple per unit volume, $\mathbf{n} \wedge \tau$ a couple stress tensor.

In these general terms, the equations are much like those associated with the EL theory, although we do have the additional equation for S . In this, the consensus of opinion is that, for at least most purposes, the “molecular inertia” terms are negligible. I'll accept this, assuming that $P \equiv 0, \pi \equiv 0$. From (3.15), one can see that there is then no loss in generality in assuming that

$$(3.21) \quad \varphi = \varphi(S, \nabla S, \mathbf{n}, \nabla \mathbf{n}, \theta), a \equiv 0,$$

which simplifies matters a bit. It then follows from our assumptions that constitutive equations for φ, σ *etc.* are objective.

Following the pattern of theories mentioned earlier, we specialize more, to theory of the “near equilibrium” kind, assuming that the constitutive functions for $\hat{\sigma}, \hat{G}, \hat{\mathbf{g}}$ and $\hat{\mathbf{q}}$ are linear in the variables which vanish in equilibrium, *viz.*

$$(3.22) \quad \dot{S}, \dot{\mathbf{n}}, \nabla \mathbf{v}, \nabla \theta,$$

with coefficients depending on

$$(3.23) \quad S, \mathbf{n}, \theta,$$

but not on $\nabla \mathbf{n}$ or ∇S . There, from (3.16), Δ becomes an homogeneous quadratic function of the variables in (3.22), with coefficients depending on those in (3.23).

With these assumptions, the matter of determining what forms of the constitutive equations are consistent with invariance assumptions has almost been done for us, by Leslie [20]. This includes objectivity, and a bit more. He assumes, as is consistent with experience, that the equations are invariant under the transformation $\mathbf{n} \rightarrow -\mathbf{n}$. From our view this can be viewed as one implication of the idea that the basic variable is \mathbf{Q} , one which is consistent with experience. For nematics, but not cholesterics, constitutive equations should be invariant under improper as well as proper or transformations. We will focus on the nematics, noting the differences for cholesterics at the end of this paper. I won't belabor the relatively simple invariance problems associated with the additional terms which arise, because S is now variable.

Insofar as possible, I'll use labelling of moduli given by Leslie [20]. To within terms which can be absorbed in Lagrange multipliers, I get

$$(3.24) \quad \begin{aligned} \hat{\sigma} = & (\beta_1 \dot{S} + \alpha_1 \mathbf{n} \cdot \mathbf{A} \mathbf{n}) \mathbf{n} \otimes \mathbf{n} + \alpha_2 \mathbf{N} \otimes \mathbf{n} + \alpha_3 \mathbf{n} \otimes \mathbf{N} \\ & + \alpha_4 \mathbf{A} + \alpha_5 \mathbf{A} \mathbf{n} \otimes \mathbf{n} + \alpha_6 \mathbf{n} \otimes \mathbf{A} \mathbf{n}. \end{aligned}$$

Here, the α 's and β 's can still depend on S and θ , and we use the notation

$$(3.25) \quad \begin{cases} 2\mathbf{A} &= \nabla \dot{\mathbf{v}} + \nabla \dot{\mathbf{v}}^T, \\ 2\mathbf{\Omega} &= \nabla \dot{\mathbf{v}} - \nabla \dot{\mathbf{v}}^T, \\ \mathbf{N} &= \dot{\mathbf{n}} - \mathbf{\Omega} \mathbf{n}. \end{cases}$$

Similarly, we have

$$(3.26) \quad \begin{cases} \hat{\mathbf{g}} = -\gamma_1 \mathbf{N} - \gamma_2 \mathbf{A} \mathbf{n}, \gamma_1 = \alpha_3 - \alpha_2, \gamma_2 = \alpha_6 - \alpha_5, \\ \hat{G} = -\beta_2 \dot{S} - \beta_3 \mathbf{n} \cdot \mathbf{A} \mathbf{n}, \\ \mathbf{q} = K_1 \nabla \theta + K_2 \nabla \theta \cdot \mathbf{n} \mathbf{n}, \end{cases}$$

the three β 's being moduli not occurring in the EL theory. I do prefer a different labelling, to be introduced shortly, but record this, because it better fits rather common practice. From (3.14) these, together with a specification of the constitutive equation for φ , determine all of the constitutive functions. We will consider φ later.

From here on, we have two aims, not unrelated. One is to explore what else might be said about the constitutive equations, based on fairly general ideas about molecular theory. Also, for the defects, we would like to know something about how the constitutive equations behave near them, that is for S near zero.

4. Onsager relations. Loosely related to molecular theory are Onsager relations. Being mindful of criticisms such as are covered by Truesdell [24, Lect 7], I do have qualms about their applicability. In the liquid crystal area, in particular, there has been a little confusion about what they are, as is discussed by Lam [25]. I will give my interpretation

of what they are, and make some use of them. The first step is to put (3.16) in a slightly different form, writing it as a bilinear form

$$(4.1) \quad 2\mathcal{D} \stackrel{def}{=} \Delta = tr(\nabla \mathbf{v} \hat{\sigma}^T) + \mathbf{h} \cdot \dot{\mathbf{n}} + H \dot{S} + \mathbf{k} \cdot \nabla \theta,$$

where

$$\mathbf{h} = -\hat{\mathbf{g}}, \quad H = -\hat{G}, \quad \mathbf{k} = -\mathbf{q}/\theta.$$

As I interpret the relations, it is not relevant which of the entries are called forces or fluxes. What is of import is how the terms transform under time reversals. To remember what to do, I find it easier to divide the variables into two groups which behave similarly. As I interpret,

$$(4.3) \quad \nabla \mathbf{v}, \dot{\mathbf{n}}, \dot{S} \text{ and } \mathbf{k} \text{ reverse sign ,}$$

whereas $\hat{\sigma}, \mathbf{h}, H$ and $\nabla \theta$ don't. If we were to regard $\hat{\sigma}, \mathbf{h}, H$ and $\nabla \theta$ as linear functions of $\nabla \mathbf{v}, \dot{\mathbf{n}}, \dot{S}$ and \mathbf{k} , with coefficients depending on S, θ and \mathbf{n} , the Onsager relations would be equivalent to the statement that, to within terms of the Lagrange multiplier kind,

$$(4.4) \quad \hat{\sigma} = \frac{\partial \mathcal{D}}{\partial \nabla \mathbf{v}}, \mathbf{h} = \frac{\partial \mathcal{D}}{\partial \dot{\mathbf{n}}}, H = \frac{\partial \mathcal{D}}{\partial \dot{S}}, \nabla \theta = \frac{\partial \mathcal{D}}{\partial \mathbf{k}}.$$

It is in fact rather awkward to use \mathbf{k} as an independent variable, instead of $\nabla \theta$. However, we can interchange these, by the usual device of introducing a Lagendre transform, *viz.*

$$(4.5) \quad \overline{\mathcal{D}} = \mathcal{D} - \mathbf{k} \cdot \frac{\partial \mathcal{D}}{\partial \mathbf{k}} = \mathcal{D} - \mathbf{k} \cdot \nabla \theta.$$

In terms of this, we have

$$(4.6) \quad \hat{\sigma} = \frac{\partial \overline{\mathcal{D}}}{\partial \nabla \mathbf{v}}, \mathbf{h} = \frac{\partial \overline{\mathcal{D}}}{\partial \dot{\mathbf{n}}}, H = \frac{\partial \overline{\mathcal{D}}}{\partial \dot{S}}, \mathbf{k} = -\frac{\partial \overline{\mathcal{D}}}{\partial \nabla \theta}.$$

Reverting to earlier notation, we then have

$$(4.7) \quad 2\overline{\mathcal{D}} = tr(\nabla \mathbf{v} \hat{\sigma}^T) - \hat{\mathbf{g}} \cdot \dot{\mathbf{n}} - \hat{G} \dot{S} + \mathbf{q} \cdot \nabla \theta / \theta$$

with

$$(4.8) \quad \hat{\sigma} = \frac{\partial \overline{\mathcal{D}}}{\partial \nabla \mathbf{v}}, \hat{\mathbf{g}} = -\frac{\partial \overline{\mathcal{D}}}{\partial \dot{\mathbf{n}}}, \hat{G} = -\frac{\partial \overline{\mathcal{D}}}{\partial \dot{S}}, \mathbf{q} = \theta \frac{\partial \overline{\mathcal{D}}}{\partial \nabla \theta},$$

which can be applied to nematics or cholesterics. For (4.4) and (4.8), one obviously needs some invertibility. Here this is not a very serious worry, but (4.8) might be considered as more natural, given our ideas about constitutive equations. If I correctly understand

remarks made by Lam [25], he accepts the equivalent of (4.4) for cholesterics, but was unsure how to proceed, if he started with $\nabla\theta$ instead of \mathbf{k} or \mathbf{q} , as an independent variable.

Comparing (4.8) with (3.24-26), I get two relations

$$(4.9) \quad \begin{cases} \gamma_2 = \alpha_2 + \alpha_3, \\ \beta_1 = \beta_3, \end{cases}$$

the former occurring in the EL theory as Parodi's relation. It is rather widely accepted, although experimentists seem not to have tried to determine whether it holds accurately. According to Currie [26], some curious instabilities are predicted, if it fails. I would find it comforting to see some similar reason for accepting the latter equality, finding arguments favoring these relations rather shakey. Kuzuu and Doi [3] do note that the former is predicted by the type of molecular theory which they explore, enough to indicate that there are molecular theories producing at least one of the two relations.

When (4.9) holds, one can use (3.16) and (3.24-26) to calculate that

$$(4.10) \quad \begin{aligned} \Delta = & \alpha_4 tr \mathbf{A}^2 + (\alpha_5 + \alpha_6) \mathbf{n} \cdot \mathbf{A}^2 \mathbf{n} + \alpha_1 (\mathbf{n} \cdot \mathbf{A} \mathbf{n})^2 \\ & + \gamma_1 |\mathbf{N}|^2 + 2\gamma_2 \mathbf{N} \cdot \mathbf{A} \mathbf{n} + \beta_2 \dot{S}^2 + 2\beta_1 \dot{S} \mathbf{n} \cdot \mathbf{A} \mathbf{n} \\ & - K_1 |\nabla\theta|^2 - K_2 (\nabla\theta \cdot \mathbf{n})^2. \end{aligned}$$

This should be non-negative and, for the present, I assume that it is, in the strict sense. One can get the related inequalities to be satisfied by scalar moduli by reducing this to a sum of independent quadratics. To do so, I introduce the projection operator

$$(4.11) \quad \mathbf{P} = 1 - \mathbf{n} \otimes \mathbf{n}.$$

Bear in mind that, from (3.1) and (3.2), $tr \mathbf{A} = 0$. Let

$$(4.12) \quad \begin{aligned} \mathbf{B} = & \mathbf{A} + \frac{1}{2} \mathbf{n} \cdot \mathbf{A} \mathbf{n} 1 - \mathbf{n} \otimes \mathbf{P} \mathbf{A} \mathbf{n} - \mathbf{P} \mathbf{A} \mathbf{n} \otimes \mathbf{n} \\ & - \frac{3}{2} \mathbf{n} \cdot \mathbf{A} \mathbf{n} \mathbf{n} \otimes \mathbf{n}, \end{aligned}$$

which satisfies

$$(4.13) \quad \mathbf{B} = \mathbf{B}^T, \mathbf{B} \mathbf{n} = 0, tr \mathbf{B} = 0.$$

Solving (4.12) for \mathbf{A} gives a good decomposition of \mathbf{A} into parts, associated with planes having \mathbf{n} as normal. In particular, a calculation gives

$$tr \mathbf{A}^2 = tr \mathbf{B}^2 + (\mathbf{n} \cdot \mathbf{A} \mathbf{n})^2 + |\mathbf{P} \mathbf{A} \mathbf{n}|^2$$

It is easy enough to check that one can choose \mathbf{A} and so that any two of the three terms on the right vanishes, with the third being non-zero. So this expresses $tr\mathbf{A}^2$ as a sum of independent quadratics. Similarly

$$\mathbf{A}\mathbf{n} = \mathbf{P}\mathbf{A}\mathbf{n} + \mathbf{n} \cdot \mathbf{A}\mathbf{n}\mathbf{n},$$

so

$$(4.15) \quad \mathbf{n} \cdot \mathbf{A}^2 \mathbf{n} = |\mathbf{A}\mathbf{n}|^2 = |\mathbf{P}\mathbf{A}\mathbf{n}|^2 + (\mathbf{n} \cdot \mathbf{A}\mathbf{n})^2.$$

With more juggling of this kind, one can reduce Δ to the form

$$(4.16) \quad \begin{aligned} \Delta = & \eta_1 tr\mathbf{B}^2 + \eta_2 (\mathbf{n} \cdot \mathbf{A}\mathbf{n})^2 + \eta_3 |\mathbf{P}\mathbf{A}\mathbf{n}|^2, \\ & + \gamma |\mathbf{N} - \lambda \mathbf{P}\mathbf{A}\mathbf{n}|^2 + \delta (\dot{S} - \mu \mathbf{n} \cdot \mathbf{A}\mathbf{n})^2, \\ & + k_\perp |\nabla\theta - \nabla\theta \cdot \mathbf{n}\mathbf{n}|^2 + k_\parallel (\nabla \cdot \theta)^2, \end{aligned}$$

and verify that one can pick velocity fields, *etc.* so that, instantaneously at a point, just one of the seven terms on the right is non-zero. This has some heuristic value, suggesting simple experiments which might provide useful information concerning the moduli, *etc.* One then has

$$(4.17) \quad \Delta \geq 0, \text{ strictly } \Leftrightarrow \eta_n (n = 1, 2, 3), \gamma, \delta, k_\perp \text{ and } k_\parallel > 0.$$

Essentially, this is the labelling and, as I interpret it, the idea underlying this which is used by Landau *et. al.* [27, e.g. (42.8)], except that they write $\bar{\eta}_2$ in place of η_2 . I do prefer this to other labellings used, some of which are mentioned by Stephen and Straley [23]. One can adjust it, to cover the possibility that (4.9) doesn't hold, but I won't do so.

A calculation gives

$$(4.18) \quad \left\{ \begin{array}{l} \eta_1 = \alpha_4, \\ \eta_2 = \alpha_1 + 3\alpha_4/2 + \alpha_5 + \alpha_6 - \beta_1^2/\beta_2, \\ \eta_3 = 2\alpha_4 + \alpha_5 + \alpha_6 - \gamma_2^2/\gamma_1, \\ \gamma = \gamma_1, \\ \delta = \beta_2, \\ \lambda = -\gamma_2/\gamma_1, \\ \mu = -\beta_1/\beta_2, \\ k_\perp = -K_1, \\ k_\parallel = -K_1 - K_2, \end{array} \right.$$

or the inverse form

$$(4.19) \quad \left\{ \begin{array}{l} \alpha_1 = \eta_1/2 + \eta_2 - \eta_3 - \lambda^2\gamma + \mu^2\delta, \\ 2\alpha_2 = \gamma_2 - \gamma_1 = -(\lambda + 1)\gamma, \\ \alpha_3 = \gamma_1 + \gamma_2 = (1 - \lambda)\gamma, \\ \alpha_4 = \eta_1, \\ 2\alpha_5 = -2\eta_1 + \eta_3 + \lambda(\lambda + 1)\gamma, \\ 2\alpha_6 = 2(\alpha_5 + \gamma_2) = -2\eta_1 + \eta_3 + \lambda(\lambda - 1)\gamma, \\ \beta_1 = \beta_3 = -\mu\delta, \\ \beta_2 = \delta \\ \gamma_1 = \gamma, \\ \gamma_2 = -\lambda\gamma, \\ K_1 = -k_\perp, \\ K_2 = k_\perp - k_\parallel. \end{array} \right.$$

Given the special form of Δ here occurring, one can replace (4.8) by

$$(4.20) \quad \left\{ \begin{array}{l} 2\hat{\sigma} = \frac{\partial \Delta}{\partial \nabla \mathbf{v}}, \\ 2\hat{G} = -\frac{\partial \Delta}{\partial S}, \\ 2\hat{g} = -\frac{\partial \Delta}{\partial \mathbf{n}}, \\ 2\mathbf{q} = -\theta \frac{\partial \Delta}{\partial \nabla \theta}, \end{array} \right.$$

with Δ expressed in the form (4.10) or (4.16). Bear in mind that, in this section, we are not considering cholesterics, and, in fact, (4.20) does not apply to them.

By assuming that (4.9) applies, we need just two scalar constitutive equations, one for Δ and one for φ . In considerations to follow, I'll assume this, to simplify matters a bit. With some additional labor, one could work through the more general case.

5. Energetics. First, we specialize (3.21), following the pattern of theories mentioned earlier. There is the idea that, for the temperatures of interest, we are dealing with nematic phases. With this is associated the idea that φ is minimized by some nematic configuration, with $S = S_0(\theta)$ and \mathbf{n} a constant unit vector field, so

$$(5.1) \quad \begin{aligned} W(S, \nabla S, \mathbf{n}, \nabla \mathbf{n}, \theta) &\stackrel{def}{=} \varphi(S, \nabla S, \mathbf{n}, \nabla \mathbf{n}, \theta) - \varphi(S_0(\theta), 0, \mathbf{n}, 0, \theta) \\ &\geq 0. \end{aligned}$$

Also, such theories use an assumption which is reasonable if ∇S and $\nabla \mathbf{n}$ are suitably small, and is used in the rather successful OZF and EL theories: W is a quadratic function of these variables, so

$$(5.2) \quad W = W_0 + W_1 + W_2,$$

with W_0 independent of these variables, W_1 , linear in them and W_2 an homogeneous quadratic in them. Near defects, $\nabla \mathbf{n}$ certainly gets large, so the most obvious approach might be to try functions more nonlinear. I don't find it easy to give a clearcut reason for not going this route. So, I am letting intuition guide me, strongly, to take a different path. With \mathbf{n} physically equivalent to $-\mathbf{n}$, we should have

$$(5.3) \quad W(S, \nabla S, \mathbf{n}, \nabla \mathbf{n}, \theta) = W(S, \nabla S, -\mathbf{n}, -\nabla \mathbf{n}, \theta).$$

For nematics, but not cholesterics, W should also be invariant under reflections, in particular central inversions, giving the conditions

$$(5.4) \quad W(S, \nabla S, \mathbf{n}, \nabla \mathbf{n}, \theta) = W(S, -\nabla S, -\mathbf{n}, \nabla \mathbf{n}, \theta),$$

and it isn't hard to show that this combination of conditions implies that

$$(5.5) \quad W_1 = 0.$$

Of course, W should also be invariant under the group of rotations. Since a rotation can be found, mapping one unit vector to any other, this implies that W_0 is independent of \mathbf{n} and, with (5.1), we should have

$$(5.6) \quad W_0(S, \theta) \geq W_0(S_0(\theta), \theta) = 0.$$

Physically, S is only meaningful for $S \in [-1/2, 1]$, from (2.5). At $S = 1$, one has the perfectly oriented systems and, at $S = -1/2$, one has all the molecular directions perpendicular to \mathbf{n} . The notion that these are unlikely to be attained suggests the assumption that

$$(5.7) \quad \lim_{S \rightarrow -1/2} W_0(S, \theta) = \lim_{S \rightarrow 1} W_0(S, \theta) = \infty,$$

and this should at least help keep S within its allotted bounds. However, I don't know of clear evidence that it is important to assume this. As I interpret, the OZF and EL theories presume that $S = S_0(\theta)$, always, making it irrelevant to consider the function W_0 . If some one has designed experiments to determine it, I don't know of this. In any event, we here have a kind of elastic energy not occuring in the OZF or EL theories.

When $\nabla S = 0$, the possible forms of W_2 can be read off from the analysis of Frank [28], for the OZF theory, and it is not hard to determine the additional terms occuring when $\nabla S \neq 0$. Omitting details, one finds that W_2 is of the form

$$(5.8) \quad \begin{aligned} 2W_2 = & K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \text{curl } \mathbf{n})^2 + K_3|\mathbf{n} \wedge \text{curl } \mathbf{n}|^2 \\ & + (K_2 + K_4)[\text{tr } \nabla \mathbf{n}^2 - (\nabla \cdot \mathbf{n})^2] + L_1|\nabla S|^2 \\ & + L_2(\nabla S \cdot \mathbf{n})^2 + L_3\nabla \cdot \mathbf{n} \nabla S \cdot \mathbf{n} + L_4\nabla S \cdot (\nabla \mathbf{n} \mathbf{n}), \end{aligned}$$

where the K 's and L 's are functions of S and θ . The labelling of the K 's corresponds to what is now rather commonly used, for the OZF theory. Rather commonly, liquid crystal workers regard as equivalent two such functions if their difference can be written as the divergence of some vector. The likely prospects are associated with the identity

$$(5.9) \quad \begin{aligned} \nabla \cdot [f(\nabla \mathbf{n} \mathbf{n} - \nabla \cdot \mathbf{n} \mathbf{n})] &= f[tr \nabla \mathbf{n}^2 - (\nabla \cdot \mathbf{n})^2] \\ &+ \nabla f \cdot (\nabla \mathbf{n} \mathbf{n} - \nabla \cdot \mathbf{n} \mathbf{n}), \end{aligned}$$

where f is any smooth scalar function of position. By considering f as a function of S , one gets expressions like those occurring in (5.4).

To cover inequalities implied by (5.1), it helps to arrange terms a bit, as we did for Δ . Assuming that the inequalities are strict, we can write W_2 in the form

$$(5.10) \quad \begin{aligned} 2W_2 &= \overline{K}_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \text{curl } \mathbf{n})^2 + \overline{K}_3|\mathbf{n} \wedge \text{curl } \mathbf{n}|^2 \\ &+ (K_2 + K_4)[tr \nabla \mathbf{n}^2 - (\nabla \cdot \mathbf{n})^2] + K_5|\nabla S - \nabla S \cdot \mathbf{n} \mathbf{n} - \nu \nabla \mathbf{n} \mathbf{n}|^2 \\ &+ K_6(\nabla S \cdot \mathbf{n} - \sigma \nabla \cdot \mathbf{n})^2, \end{aligned}$$

where

$$(5.11) \quad \left\{ \begin{array}{l} \overline{K}_1 = K_1 - \sigma^2 K_6 = K_1 - L_3^2/4(L_1 + L_2), \\ \overline{K}_3 = K_3 - \nu^2 K_5 = K_3 - L_4^2/4L_1, \\ K_5 = L_1, \\ K_6 = L_1 + L_2, \\ \nu = -L_4/2L_1, \\ \sigma = -L_3/2L. \end{array} \right.$$

Also, the first four terms are familiar from the OZF theory, so we can copy inequalities involving them, from Ericksen [29]. We get the strict inequalities as

$$(5.8) \quad \left\{ \begin{array}{l} \overline{K}_1 > 0, K_2 > |K_4|, \overline{K}_3 > 0, 2\overline{K}_1 - K_2 - K_4 > 0 \\ K_5 > 0, K_6 > 0. \end{array} \right.$$

As will become clear, the strict inequalities fail at $S = 0$ and, in exploring this, you might find it is easier to use (5.4). For the OZF theory, workers using (5.5) to get $K_2 + K_4 = 0$, effectively, obviously then tolerate loss of the strict inequality. Clearly, W and φ differ by an additive function of θ : the dependence of $\varphi(S_0(\theta), 0, \mathbf{n}, 0, \theta)$ on \mathbf{n} being excluded by invariance. This is, of course, involved in describing specific heats, but, otherwise, there is little to be said about it.

Apart from some considerations associated with molecular theory, the format for these theories is now complete. From such things as the singular perturbation theory mentioned before, there is some suggestion that the ELP theory represents some approximation to

this. Left to itself, in a heat bath at constant temperature, we can reasonably argue that it will adopt a configuration minimizing W . So, S will take the value $S_0(\theta)$, \mathbf{n} becoming a constant unit vector. For the latter, the liquid crystal has no reason to prefer one direction over another. so, at the first step in a perturbation theory which might treat various weak influences, we have this indeterminacy. Experience with such situations suggests that the next step should be to eliminate this indeterminacy, leaving $S = S_0(\theta)$. The OZF and EL equations suggest themselves, as candidates for equations to be used at this step. Certainly, I would like to know whether rigorous asymptotic theory confirms this, or suggests some modification. I am, after all, fishing for a modification to better handle defects, things occurring on sets of measure zero. For exploring this, the present format seems to me to be about as good as the more complicated equations considered by MacMillan [11]. At the next step, I would expect the equality $S = S_0(\theta)$ to be relaxed. This could occur with or without the introduction of biaxial nematic configurations. As I see it, this is the place to consider the more general theory, to try to assess which is the more likely possibility, which would depend on the form of such equations. Clearly, there is more opinion than fact in these remarks. I am aware that various workers interested in the polymers have somewhat contrary opinions: more rigorous analyses could help clear the air.

6. Consistency conditions for W_0 . So far, we have pretty well ignored the role played by the second order tensor \mathbf{Q} , discussed in § 2. Primarily, I will use ideas about it to get estimates of the behavior of constitutive equations near $S = 0$, expecting that this will be of some import in analyses of defects. The idea is to regard constitutive equations for W and Δ as restrictions to nematic configurations of constitutive equations applicable to the more general variety of configurations. The assumption is that they are smooth near $\mathbf{Q} = 0$. For W_0 , we then start with a constitutive equation of the form

$$\overline{W}_0(\mathbf{Q}, \theta),$$

invariant under the orthogonal group. As is discussed in some detail by Ericksen [19], this is expressible in terms of two scalar invariants, which can be taken as

$$(6.2) \quad \begin{cases} J \stackrel{def}{=} \text{tr} \mathbf{Q}^2 / 6 \geq 0, \\ K \stackrel{def}{=} (\det \mathbf{Q}) / 2, \end{cases}$$

these satisfying

$$(6.3) \quad K^2 \leq J^3,$$

for real \mathbf{Q} . Here the equality holds for nematic configurations if $J \neq 0$, $J = 0$ giving the isotropic configuration. When \mathbf{Q} has the nematic form given by (2.5), a calculation gives

$$(6.4) \quad K = S^3 / 27, J = S^2 / 9.$$

To correct an erroneous statement in the above reference, I'll sketch the calculation of another relevant inequality. From (2.3), it follows that relevant values of Q_1 and Q_2 fill a triangle in the $Q_1 - Q_2$ plane: points in the boundary describe places where at least one of the these eigenvalues $Q_1, Q_2, Q_3 = -(Q_1 + Q_2)$ has the value $-1/3$. By a simple calculation, the eigenvalue equation is

$$(6.5) \quad Q^3 - 3JQ - 2K = 0$$

so

$$(6.6) \quad Q = -\frac{1}{3} \Leftrightarrow J - 2K = 1/27.$$

thus, the boundary of the triangle maps to this line in the $J - K$ plane. One has

$$(6.7) \quad J - 2K = \frac{1}{6}[Q_1^2 + Q_2^2 + (Q_1 + Q_2)^2] + Q_1 Q_2 (Q_1 + Q_2).$$

By applying derivative tests for extremals, one can show that this attains a minimum at $\mathbf{Q} = 0$, and a maximum on the boundary of the triangle. Thus, it takes on all values in the interval

$$(6.8) \quad 0 \leq J - 2K \leq 1/27.$$

By inspecting the level curves for J in this plane, one can verify that this, together with (6.3), define the physically meaningful domain for \overline{W}_0 , considered as a function of J and K . When (6.6) holds, \overline{W}_0 might reasonably be infinite, these values corresponding to the cases where the molecules are all parallel or parallel to a plane. Otherwise, I'll assume it is smooth. If it is near $\mathbf{Q} = 0$, we should have

$$(6.9) \quad \overline{W}_0 \cong aJ + o(|\mathbf{Q}|^2),$$

with a some function of θ . To get $W_0(S, \theta)$, we'll simply replace J and K by the functions of S given by (6.4). Clearly, this does not produce strong limitations on the function $W_0(S, \theta)$, but we do get, from (6.9), for $S \rightarrow 0$,

$$(6.10) \quad W_0(S, \theta) = o(S^2),$$

If, in (6.9), $a > 0$, then \overline{W}_0 will have atleast a relative minimum at $\mathbf{Q} = 0$, an isotropic phase which is at least metastable. This is likely for θ near the isotropic-nematic phase transition, and I don't feel comfortable about using our theory in such situations. However, analyses such as are given by Maddocks [14], among others, seem to indicate that having a suitably shallow "energy well" here produces predictions much like those occurring when

it is absent. Physically this is also not unreasonable. Well within the nematic range, I would expect to have $a < 0$. From discussions with experts, *etc.* the “bi-phasic” regime seems to be restricted to a narrow temperature band, so a might well become negative just a few degrees below the phase transition temperature. Similarly, at low enough temperatures, one generally encounters other “near-transition” complications, associated with the appearance of smectic phases. Here, I refer to pure substances, the so-called thermotropic liquid crystals. In solutions, concentration plays a similar role, the more dilute solutions being isotropic, *etc.* In these, one can also encounter other complications, for example phase separation.

Particularly, those involved with the polymers have needed to introduce $\overline{W}_0(\mathbf{Q}, \theta)$, generally guessing it to be some simple function. This is really what is done in some molecular theories of the “mean-field” kind, for example that used by Fan [9]. Doi [10] does briefly mention some possibilities for using available molecular theory to get more complex functions.

There are the situations of physical interest, involving electromagnetic fields, for which one needs at least crude estimates of the related field energies. For this, one can use the obvious restrictions of functions discussed by Gramsbergen *et al* [32]. More general formulations are discussed by Longa *et al* [29].

7. Consistency conditions for W_0 . here again, the implications of the idea that \mathbf{Q} is the more basic variable seem to be most restrictive for S near zero. On the other hand, there is some tendency to assume that the constitutive equations really are polynomials of low degree. It is then of some interest to know how low the degree can be, and not involve some prediction obviously contradicted by known experimental findings. So, I will try to accomodate both desires. The basic idea is that W_2 is a homogeneous quadratic polynomial in $\nabla \mathbf{Q}$, with coefficients which depend on θ , and are polynomials of low degree in \mathbf{Q} , these functions being invariant under the orthogonal group. By taking restrictions of these, we’ll get some subset described of the equations described by (5.4), say. Energy functions of interest have been characterized by Longa *et al* [30], so it is more a matter of calculating and commenting on restrictions.

For the terms of lowest degree, independent of \mathbf{Q} , there are three possible terms

$$(7.1) \quad \begin{cases} I_1 = Q_{ij,i} Q_{kj,k}, \\ I_2 = Q_{ij,k} Q_{ij,k}, \\ I_3 = Q_{ij,k} Q_{ik,j}, \end{cases}$$

in Cartesian tensor notation. With the slight rearrangement

$$(7.2) \quad \overline{W}_2 = B_1(I_3 - I_1) + B_2(3I_1 - \frac{1}{2}I_2) + B_3(2I_2 - 3I_1),$$

a somewhat tedious calculation gives, for the restrictions

$$\begin{aligned}
(7.3) \quad W_2^0 = & (B_2 - B_3)(\nabla S \cdot \mathbf{n})^2 + B_3|\nabla S|^2 \\
& + 2(2B_2 - B_1 - 2B_3)S\nabla \cdot \mathbf{n}\nabla S \cdot \mathbf{n} \\
& + 2(B_1 - B_2 + B_3)S\nabla S \cdot (\nabla \mathbf{n}\mathbf{n}) \\
& + (2B_2 + B_3)S^2[(\nabla \cdot \mathbf{n})^2 + |\mathbf{n} \wedge \text{curl } \mathbf{n}|^2] \\
& + (4B_3 - B_2)S^2(\mathbf{n} \cdot \text{curl } \mathbf{n})^2 \\
& + (B_1 - B_2 + 4B_3)S^2[\text{tr} \nabla \mathbf{n}^2 - (\nabla \cdot \mathbf{n})^2],
\end{aligned}$$

with the superscript zero indicating that this is of degree zero in \mathbf{Q} . Comparing this with (5.4), we have, in particular,

$$\begin{cases} K_1 = K_3 = 2(2B_2 + B_3)S^2, \\ K_2 = 2(4B_3 - B_2)S^2, \\ K_4 = 2B_1S^2. \end{cases}$$

It is easy to check that the strict inequalities (5.8) fail at $S = 0$. To compare with the OZF theory, consider S as a non-zero constant. Then this estimate of W_2 is a bit more flexible than the molecular theory used by Nehring and Saupe [3.1], which does give $K_1 = K_3$ and also fixes the ratio K_2/K_1 . So also does that used by Fan [9]. Longa *et al* [30] discuss more recent versions of molecular theory. Experimentally, $K_3/K_1 \neq 1$, this ratio varying quite a bit, depending on the material and temperature. So, one needs some more general function, to avoid this obvious contradiction. Special forms of W_2 used by Hardt [12] and Lin [13] are not completely consistent with (7.3), being chosen, in part, to permit use of some analytical tricks. If one is only interested in the behavior near defects where, hopefully, $S \approx 0$, this estimate might be good enough. However, it won't hurt to consider terms linear in \mathbf{Q} . It doesn't take much work to find that, nominally, there are the seven possible terms, given by

$$(7.5) \quad \begin{cases} J_1 = Q_{ij}Q_{ij,h}Q_{hp,p}, \\ J_2 = Q_{ij}Q_{ip,p}Q_{jq,q}, \\ J_3 = Q_{ij}Q_{ip,q}Q_{jq,p}, \\ J_4 = Q_{ij}Q_{ip,j}Q_{pq,q}, \\ J_5 = Q_{ij}Q_{ip,q}Q_{jp,q}, \\ J_6 = Q_{ij}Q_{ip,q}Q_{pq,j}, \\ J_7 = Q_{ij}Q_{pq,i}Q_{pq,j}. \end{cases}$$

It is not immediately obvious, but Longa *et al* [29] assert that these are not all independent, but are connected by one linear relation. By another method, I have checked this, finding that

$$(7.6) \quad 2J_1 - J_2 - J_3 - 2J_4 + 2J_5 - 2J_6 + J_7 = 0.$$

Logically, it is possible that more relations might be satisfied by the restrictions, but my calculations indicate that this is not the case. Calculating the restriction of a linear combination of such terms, I get a function of the form

$$(7.7) \quad \begin{aligned} W_2^1 = & S[C_1(\nabla S \cdot \mathbf{n})^2 + C_2|\nabla S|^2 + C_3 S \nabla \cdot \mathbf{n} \nabla S \cdot \mathbf{n} \\ & + C_4 S \nabla S \cdot (\nabla \mathbf{n} \mathbf{n}) + C_5 S^2 (\nabla \cdot \mathbf{n})^2 + C_6 S^2 \text{tr}(\nabla \mathbf{n}^2) \\ & + C_7 S^2 |\nabla \mathbf{n} \mathbf{n}|^2 + C_8 S^2 |\nabla \mathbf{n}|^2], \end{aligned}$$

where the C 's are functions of θ , restricted by two equations, *viz.*

$$(7.8) \quad \begin{cases} 18C_1 - 9C_3 - 6C_4 + 2C_5 - C_6 - 6C_7 = 0, \\ 54C_2 + 9C_3 + 6C_4 - 14C_5 - 11C_6 - 6C_7 - 36C_8 = 0. \end{cases}$$

It isn't hard to check that an energy function of the form $W_2 = W_2^0 + W_2^1$ can give $K_1 \neq K_3$, eliminating the obvious contradiction with experiment. According to Longa *et al* [30], the corresponding polynomial of next highest degree, quadratic in \mathbf{Q} , gives thirteen independent terms. I have not checked it, but it seems rather likely that, for this and higher order polynomials, the scheme imposes no limitations on the restriction, beyond what is obvious from the fact that one is dealing with polynomials of known degree.

One can regroup some terms to form divergences, as indicated by (5.5). For the number of such combinations, I get the same as do Longa *et al* [30] for the more general theory: one for W_2^0 and two for W_2^1 .

8. Consistency conditions for Δ . For Δ , we start with the assumption that it is an objective function, implying that it is reducible to a quadratic function of $\nabla\theta$ and two symmetric, traceless objective tensors. These can be taken as \mathbf{A} , given by (3.25), and¹

$$(8.1) \quad \hat{\mathbf{Q}} = \dot{\mathbf{Q}} - \Omega \mathbf{Q} + \mathbf{Q} \Omega,$$

the co-rotational time derivative used by MacMillan [11], for example. In the quadratic, the coefficients can depend on \mathbf{Q} and θ . The potential function $\overline{\mathcal{D}}$ given by (4.5) is subject to the same invariance requirements, so it will be of the same general form. Again, our concern is with the polynomials of lower degree, to estimate the behavior of constitutive equations as $S \rightarrow 0$. To get all the terms known to be relevant from experience with the ELP theory, one needs to consider polynomials quadratic in \mathbf{Q} , so this seems to be a good

¹Some workers like to use other objective tensors, differing from $\hat{\mathbf{Q}}$ by terms linear in \mathbf{Q} and in \mathbf{A} . The general theory does not favor one such over another, it being a matter of grouping terms in different ways.

place to stop. For this, I get the relevant terms as

$$(8.2) \quad \left\{ \begin{array}{l} tr \mathbf{A}^2, \\ 3tr(\mathbf{A}^2 \mathbf{Q}) = S(3\mathbf{n} \cdot \mathbf{A}^2 \mathbf{n} - tr \mathbf{A}^2), \\ 3tr \mathbf{Q}^2 tr \mathbf{A}^2 = 2S^2 tr \mathbf{A}^2, \\ 9tr(\mathbf{Q} \mathbf{A})^2 = S^2[9(\mathbf{n} \cdot \mathbf{A} \mathbf{n})^2 - 6\mathbf{n} \cdot \mathbf{A}^2 \mathbf{n} + tr \mathbf{A}^2], \\ 9tr(\mathbf{Q}^2 \mathbf{A}^2) = S^2[3\mathbf{n} \cdot \mathbf{A}^2 \mathbf{n} + 2tr \mathbf{A}^2], \\ 3tr \hat{\mathbf{Q}}^2 = 2(\dot{S}^2 + 3S^2 |\mathbf{N}|^2), \\ 9tr(tr(\hat{\mathbf{Q}}^2 \mathbf{Q}) = 2S(\dot{S}^2 + 3S^2 |\mathbf{N}|^2), \\ 9tr \mathbf{Q}^2 tr \hat{\mathbf{Q}}^2 = 4S^2(\dot{S}^2 + 3S^2 |\mathbf{N}|^2), \\ tr(\mathbf{Q} \hat{\mathbf{Q}} - \hat{\mathbf{Q}} \mathbf{Q})^2 = -2S^4 |\mathbf{N}|^2, \\ tr \mathbf{A} \hat{\mathbf{Q}} = \dot{S} \mathbf{n} \cdot \mathbf{A} \mathbf{n} + 2S \mathbf{n} \cdot \mathbf{A} \mathbf{N}, \\ 3tr(\mathbf{A} \mathbf{Q} \hat{\mathbf{Q}}) = S(\dot{S} \mathbf{n} \cdot \mathbf{A} \mathbf{n} + S \mathbf{n} \cdot \mathbf{A} \mathbf{N}), \\ 3tr \mathbf{Q}^2 tr \mathbf{A} \hat{\mathbf{Q}} = 2S^2(\dot{S} \mathbf{n} \cdot \mathbf{A} \mathbf{n} + 2S \mathbf{n} \cdot \mathbf{A} \mathbf{N}), \\ 9tr(\mathbf{Q}^2 \mathbf{A} \hat{\mathbf{Q}}) = S^2(3\dot{S} \mathbf{n} \cdot \mathbf{A} \mathbf{n} + 5S \mathbf{n} \cdot \mathbf{A} \mathbf{N}), \\ |\nabla \theta|^2, \\ 3\nabla \theta \cdot \mathbf{Q} \nabla \theta = S[3(\nabla \theta \cdot \mathbf{n})^2 - |\nabla \theta|^2], \\ 3tr \mathbf{Q}^2 |\nabla \theta|^2 = 2S^2 |\nabla \theta|^2, \\ 3\nabla \theta \cdot \mathbf{Q}^2 \nabla \theta = S^2[3(\nabla \theta \cdot \mathbf{n})^2 - |\nabla \theta|^2], \end{array} \right.$$

where \mathbf{N} is given by (3.25). For more general forms of \mathbf{Q} , one should add two terms, which can be taken as $tr(\mathbf{Q} \mathbf{A} \mathbf{Q} \mathbf{A} \hat{\mathbf{Q}})$ and $tr(\mathbf{Q}^2 \hat{\mathbf{Q}}^2)$, which here reduced to combinations of terms already listed.² Multiplying the first term in (8.2) by A_1 , the second by A_2 *etc.*, and adding them up, we get an estimate of Δ of the form (4.10), with

$$(8.3) \quad \left\{ \begin{array}{l} \alpha_1 = 9A_4 S^2, \\ \alpha_4 = A_1 - A_2 S + 2A_3 S^2 + A_4 S^2 + 2A_5 S^2, \\ \alpha_5 + \alpha_6 = 3A_2 S - 6A_4 S^2 + 3A_5 S^2, \\ \gamma_1 = 2S^2(3A_6 + 3A_7 S + 6A_8 S^2 - A_9 S^2), \\ 2\gamma_2 = S(2A_{10} + A_{11} S + 4A_{12} S^2 + 5A_{13} S^2), \\ \beta_2 = 2(A_6 + A_7 S + 2A_8 S^2), \\ 2\beta_1 = A_{10} + A_{11} S + 2A_{12} S^2 + 3A_{13} S^2, \\ -K_1 = A_{14} - A_{15} S + 2A_{16} S^2 - A_{17} S^2, \\ -K_2 = 3A_{15} S + 3A_{17} S^2. \end{array} \right.$$

² Relevant representation theorems for polynomials of arbitrary degree are presented by Smith [33], for example. Wang [34] considers more general functions.

Here the A 's depend on θ only. As might be expected, the strict inequalities indicated by (4.17) and (4.18) can't hold at $S = 0$, although weaker versions can still hold. Pragmatically, it would be hard to find experiments contradicting the idea that Δ is representable in this form for all relevant values of S . Berry [35] presents results of calculations based on molecular theories for lyotropic liquid crystals (solutions). These give functions which are a bit more complicated but behave similarly, for S near zero. As might be expected, different molecular theories give different functions. It seems premature to try to discuss how best to select the various functions of S and θ which are involved in these theories but, certainly, this is a knotty problem. It is unrealistic to think that they could all be determined by experiment.

9. Cholesterics. Formally, the analogous theory for cholesteric liquid crystals involves some additional terms, roughly those which are invariant under rotations, but not reflections. I'll not discuss these in detail, but will record the differences. For the energy W , the energies W_0 and W_2 have the same form as for nematics but, instead of being zero, W_1 can now be of the form

$$(9.1) \quad W_1 = M(S, \theta) \mathbf{n} \cdot \text{curl } \mathbf{n}.$$

For $S \rightarrow 0$, one gets the asymptotic form

$$(9.2) \quad M = B(\theta)S^2 + \hat{B}(\theta)S^3 + o(S^3).$$

Physically, W should be bounded below, which requires that

$$(9.3) \quad W_2 \geq 0, W_2 = 0 \Rightarrow W_1 = 0$$

Usually, workers assume that W is minimized by configurations with S a positive constant or, more realistically, some function of θ , and for \mathbf{n} of the form

$$(9.4) \quad \mathbf{n} = (\cos \tau z, \sin \tau z, 0),$$

in some rectangular Cartesian coordinate system, with τ a function of θ . In considering so-called blue phases, Sethna [8] discusses cases of "frustration", where no unit vector field minimizes W . In these, one encounters more or less periodic arrays of line singularities which should be mollified a bit, for a satisfactory mathematical theory. In the more common phases to which (9.4) applies, line defects also occur. Also, if W is minimized by a field of the form (9.4), Jenkins [36] notes that the OZF moduli must satisfy

$$(9.5) \quad K_2 + K_4 = o,$$

and suggests a more nonlinear function of $\nabla \mathbf{n}$ to better describe configurations near such minimizers. However, most workers seem to be content using the quadratic, commonly

accepting (9.5) for the different reason discussed in § 5. This is the coefficient of a term which can be written as a divergence, when S and θ are constant. Predictions obtained from the simpler form seem good enough to satisfy workers, in general.

For simplicity, I'll again assume that the Onsager relations apply, so one can calculate non-equilibrium parts of the stress tensor, *etc.*, using (4.6), if one knows the scalar function $\overline{\mathcal{D}}$. A part of this, say $\overline{\mathcal{D}}_N$, has the same form as for a nematic, so it is only necessary to specify the form of the remainder

$$(9.6) \quad \mathcal{D}_c = \overline{\mathcal{D}} - \overline{\mathcal{D}}_N.$$

One finds that it is of the form

$$(9.7) \quad \mathcal{D}_c = T(S, \theta) \nabla \theta \cdot \mathbf{n} \wedge \mathbf{A} \mathbf{n} + U(S, \theta) \nabla \theta \cdot \mathbf{n} \wedge \mathbf{N}.$$

Also, for $S \rightarrow 0$, one has

$$(9.8) \quad \begin{cases} T = C(\theta)S + \hat{C}(\theta)S^2 + o(S^2), \\ U = D(\theta)S^2 + o(S^2). \end{cases}$$

Obviously, the terms added to W and \mathcal{D} remain when S is a non-zero constant, so they are involved in the OZF and Leslie's [37] analogous theories for cholesterics, being in this sense familiar. However, many investigations presume that $\theta = \text{const.}$, so $\mathcal{D}_c = 0$. There is an interesting exception, involving the term multiplied by U . Briefly, a temperature gradient can cause \mathbf{n} to undergo a spinning motion. A simple analysis of this is given by Leslie [37], as an explanation of an old observation by Lehmann of "optical isotropy" induced by a temperature gradient.

This completes our presentation of the basic equations, incorporating some features suggested by molecular theories, without committing ourselves to any particular molecular theory.

For both the nematic and cholesteric types, one can avoid assuming the Onsager relations, in part, by introducing other comparable assumptions concerning stress and heat flux, considered as functions of \mathbf{Q} , $\hat{\mathbf{Q}}$ *etc.* Dealing with such things as $\hat{\mathbf{g}}$ and \hat{G} is trickier since, in the theory allowing more general variations in \mathbf{Q} , one does not have such a vector and scalar. The analogous quantity is a symmetric second order tensor, call it $\hat{\mathcal{G}}$. It is the latter which should reduce to a function of \mathbf{Q} *etc.* As I see it, the likely way of making the identification is to set

$$(9.9) \quad \hat{\mathbf{g}} = 2S\hat{\mathcal{G}}\mathbf{n}, \hat{G} = \text{tr}[\hat{\mathcal{G}}(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{1})],$$

which fits the power balance

$$(9.10) \quad \hat{\mathbf{g}} \cdot \dot{\mathbf{n}} + \hat{G}\dot{S} = \text{tr}\hat{\mathcal{G}}\dot{\mathbf{Q}},$$

for \mathbf{Q} of the nematic form. I'll not use the ink to elaborate this.

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