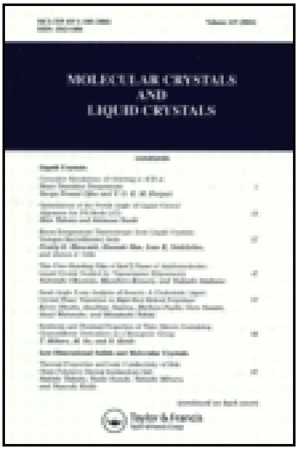

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DERIVATION OF A DIFFERENTIAL EQUATION FOR A CHOLESTERIC LIQUID CRYSTAL IN ELECTRIC FIELDS *

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Abstract   Liu's lemma and some additional equilibrium conditions are used to calculate the stress tensor of a liquid crystal in electromagnetic fields. With the resulting constitutive equations, the balance of moment of momentum in equilibrium yields the differential equation for the director field. The example of a distorted cholesteric helix is treated. The resulting equation is the same one, De Gennes[1] derived on another way.

INTRODUCTION

The differential equations determining the motion of a liquid crystal in electromagnetic fields are the mechanical balance equations:

$$\dot{\rho} + \rho \nabla_\alpha v_\alpha = 0 \qquad \text{(mass)} \qquad (1)$$

$$\dot{\rho} \underset{cm}{p}_\beta + \rho \dot{v}_\beta - \nabla_\gamma t_{\beta\gamma} - \rho f_\beta = 0 \qquad \text{(momentum)} \qquad (2)$$

$$\rho \Theta d_{[\alpha|} \ddot{d}_{|\beta]} - \nabla_\gamma m_{\alpha\beta\gamma} - l_{\alpha\beta} + t_{[\alpha\beta]} = 0 \quad \text{(moment of momentum)} \quad (3)$$

$$\rho\dot{\varepsilon} - t_{\alpha\beta} \nabla_\beta v_\alpha + \nabla_\alpha q_\alpha - 2 m_{\alpha\beta\gamma}\nabla_\gamma(\dot{d}_\beta d_\alpha) - \rho r - 2\dot{d}_\alpha d_\beta t_{[\beta\alpha]} = 0$$

(internal and electromagnetic energy) (4)

including moment, moment of momentum and energy of the electromagnetic field and the Maxwell equations

$$\nabla_\alpha D_\alpha - \underset{e}{\rho} = 0 \qquad (5)$$

* Part of the poster "ELECTROSTRICTION OF THE CHOLESTERIC BLUE PHASES BPI AND BPII" by G. HEPPKE, B. JEROME, R. ELLINGHAUS, H.-S. KITZEROW, W. MUSCHIK, CH. PAPENFUß and P. PIERANSKI

$$e_{\alpha\beta\gamma} \nabla_\beta \mathcal{H}_\gamma - \overset{*}{D}_\alpha - j_\alpha = 0 \tag{6}$$

$$e_{\alpha\beta\gamma} \nabla_\beta \mathcal{E}_\gamma + B_\alpha = 0 \tag{7}$$

$$\nabla_\alpha B_\alpha = 0 \tag{8}$$

with the objective quantities $\mathcal{E} = \underline{E} + \underline{v} \times \underline{B}$, $\mathcal{H} = \underline{H} - \underline{v} \times \underline{D}$ and the convective time derivative of a vector field $\underline{X}$, given by $\overset{*}{\underline{X}} := \dot{\underline{X}} + \underline{X}\,(\nabla \cdot \underline{v}) - \underline{X} \cdot \nabla \underline{v}$.

The remaining quantities are:

ρ: mass density, $\underline{v}$: velocity, $\underline{p}_{em}$: momentum density of the electromagnetic field, $\underline{\underline{t}}$: total stress tensor, $\underline{d}$: director, Θ: inertia of a particle, ε: sum of the densities of internal and electromagnetic energy, $\underline{q}$: conductive energy flux, $\underline{f}$: external body force, $\underline{\underline{m}}$: surface density of couple, $\underline{\underline{l}}$: density of body couple, r: absorption of radiation, ρ_e: electric charge density, $\underline{B}$: magnetic flux density, $\underline{E}$: electric field, $\underline{j}$: electric current density, $\underline{H}$: magnetic field, $\underline{D}$: dielectric displacement

A suitable choice for a state space is:

$$Z = (\rho,\ T,\ \underline{d},\ \mathcal{E},\ \underline{B},\ \nabla\rho,\ \nabla T,\ \nabla \underline{d},\ \nabla \underline{v},\ \dot{\underline{d}}) \tag{9}$$

Liu's Lemma assures the existence of Lagrange Multipliers $\Lambda_{(\cdot)}$, such that the inequality (η: entropy density, $\underline{\Phi}$: entropy flux)

$$\begin{aligned}
&\rho\dot{\eta} + \nabla_\alpha \Phi_\alpha + \Lambda_\rho \left(\dot{\rho} + \rho\, \nabla_\alpha v_\alpha \right) + \Lambda_{v\,\beta} \left[\rho\, \dot{p}_{em\beta} + \rho\, \dot{v}_\beta - \nabla_\gamma t_{\beta\gamma} - \rho f_\beta \right] + \\
&\Lambda_{d\,\alpha\beta} \left[\rho \Theta d_{[\alpha|} \ddot{d}_{|\beta]} - \nabla_\gamma m_{\alpha\beta\gamma} - l_{\alpha\beta} + t_{[\alpha\beta]} \right] + \Lambda_e \Big[\rho \dot{\varepsilon} - t_{\alpha\beta} \nabla_\beta v_\alpha + \nabla_\alpha q_\alpha \\
&- 2 m_{\alpha\beta\gamma} \nabla_\gamma (\dot{d}_\beta d_\alpha) - \dot{d}_\alpha d_\beta t_{[\beta\alpha]} \Big] + \Lambda_D \left[\nabla_\alpha D_\alpha - \rho_e \right] + \Lambda_{\mathcal{E}\,\alpha} \left[e_{\alpha\beta\gamma} \nabla_\beta \mathcal{E}_\gamma + \overset{*}{B}_\alpha \right] \\
&+ \Lambda_{H\,\alpha} \left[e_{\alpha\beta\gamma} \nabla_\beta \mathcal{H}_\gamma - \overset{*}{D}_\alpha - j_\alpha \right] + \Lambda_B \nabla_\alpha B_\alpha \geq 0
\end{aligned} \tag{10}$$

holds for all solutions of the balance equations.

CONSTITUTIVE EQUATIONS IN NONEQUILIBRIUM

After elimination of the Lagrange parameters the constitutive relations read ($f := \rho(\varepsilon - T\eta)$ and $\underline{K} := \underline{\Phi} - \frac{\underline{q}}{T}$):

$$0 = -\frac{1}{T}\frac{\partial f}{\partial X} + \frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\gamma}\frac{\partial D_\gamma}{\partial X}, \qquad X := \left(T,\ \nabla_\alpha T,\ \nabla_\alpha v_\beta,\ \nabla_\alpha \rho\right) \quad (11)$$

$$0 = \frac{\partial K_\nu}{\partial Y} - \frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\gamma} e_{\gamma\nu\delta}\frac{\partial \mathcal{H}_\delta}{\partial Y}, \quad Y := \left(\nabla_\alpha d_\beta, B_\alpha, \nabla_\alpha T, \nabla_\alpha v_\beta, \nabla_\alpha \rho\right) \quad (12)$$

$$0 = \frac{\partial K_\beta}{\partial \mathcal{E}_\alpha} + \frac{1}{T}\frac{\partial f}{\partial B_\gamma} e_{\gamma\beta\alpha} \quad (13)$$

$$0 = -\frac{1}{T}\frac{\partial f}{\partial \nabla_\alpha d_\beta} + \frac{\partial K_\alpha}{\partial d_\beta} - \frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\gamma}\left(e_{\gamma\alpha\delta}\frac{\partial \mathcal{H}_\delta}{\partial d_\beta} - \frac{\partial D_\gamma}{\partial \nabla_\alpha d_\beta}\right) + \frac{1}{T} m_{\gamma(\beta\alpha)} d_\gamma \quad (14)$$

Up to here the following assumptions have been used:

$$\Lambda_e = -\frac{1}{T} \quad (15)$$

$$\left(\frac{\partial \underline{D}}{\partial \underline{\mathcal{E}}}\right)^{-1} \text{ exists} \quad (16)$$

$$\frac{\partial \underline{\mathcal{H}}}{\partial \underline{\mathcal{E}}} = \underline{\underline{0}} = \frac{\partial \underline{D}}{\partial \underline{B}} \quad (17)$$

$\underline{\underline{\alpha}} := \dfrac{\partial \underline{D}}{\partial \underline{\mathcal{E}}}$ and $\dfrac{\partial \underline{\mathcal{H}}}{\partial \underline{B}}$ are symmetric.

With the additional assumption $\underline{K} = -\frac{1}{T}\underline{\mathcal{E}} \times \underline{\mathcal{H}}$ and the existence of $\left(\frac{\partial \underline{\mathcal{H}}}{\partial \underline{B}}\right)^{-1}$ equation (12) yields

$$\frac{\partial f}{\partial \mathcal{E}_\alpha} = \mathcal{E}_\gamma \frac{\partial D_\gamma}{\partial \mathcal{E}_\alpha} \quad (18)$$

and from equation (13) may be concluded

$$\mathcal{H}_\delta = \frac{\partial f}{\partial B_\delta} \quad (19)$$

Assuming the energy density of the electromagnetic field of Grot and Eringen[3] equations (18) and (19) coincide with the known equilibrium equations.

EQUILIBRIUM CONDITIONS FROM THE RESIDUAL DISSIPATION INEQUALITY

With the Liu equations the inequality (10) takes the form

$$N_\alpha\left[-\frac{1}{T}\frac{\partial f}{\partial d_\alpha} + \frac{2}{T} m_{\gamma\alpha\beta}\nabla_\beta d_\gamma + \frac{2}{T} d_\beta t_{[\beta\alpha]} + \frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\beta}\frac{\partial D_\beta}{\partial d_\alpha}\right] +$$

$$+\nabla_\alpha d_\beta\left[\frac{\partial K_\alpha}{\partial d_\beta}-\frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\gamma}e_{\gamma\alpha\delta}\frac{\partial \mathcal{H}_\delta}{\partial d_\beta}\right]+\nabla_{(\alpha|}v_{|\beta)}\left[\delta_{\alpha\beta}\left(\frac{\rho^2}{T}\frac{\partial(f/\rho)}{\partial\rho}\right.\right.$$
$$-\frac{\rho}{T}\frac{\partial D_\alpha}{\partial\rho}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\alpha}+\frac{1}{T}\frac{\partial f}{\partial B_\gamma}B_\gamma+\frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\gamma}D_\gamma\Big)+\frac{1}{T}t_{(\alpha\beta)}-\frac{1}{T}\frac{\partial f}{\partial B_{(\alpha|}}B_{|\beta)}$$
$$-\frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu(\alpha|}D_{|\beta)}+\nabla_{(\beta|}d_\mu\left(\frac{\partial K_\alpha}{\partial d_\mu}-\frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\nu}\alpha^{-1}_{\nu\delta}e_{\delta|\alpha)\gamma}\frac{\partial \mathcal{H}_\gamma}{\partial d_\mu}+\frac{2}{T}m_{\nu\mu|\alpha)}d_\nu\right)\Bigg]$$
$$+\nabla_\alpha\rho\left[\frac{\partial K_\alpha}{\partial\rho}-\frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\beta}e_{\beta\alpha\gamma}\frac{\partial \mathcal{H}_\gamma}{\partial\rho}\right]+\nabla_\alpha T\left[\frac{\partial K_\alpha}{\partial T}-\frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\gamma}e_{\gamma\alpha\beta}\frac{\partial \mathcal{H}_\beta}{\partial T}\right]$$
$$+w_{\beta\alpha}\left[\frac{1}{T}t_{[\alpha\beta]}-\frac{1}{T}\frac{\partial f}{\partial B_{[\alpha|}}B_{|\beta]}-\frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu[\alpha|}D_{|\beta]}+d_{[\alpha|}\left(-\frac{1}{T}\frac{\partial f}{\partial d_{|\beta]}}+\right.\right.$$
$$\left.\left.+\frac{2}{T}m_{\gamma|\beta]\mu}\nabla_\mu d_\gamma+\frac{2}{T}d_\gamma t_{\gamma|\beta]}+\frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\gamma}\frac{\partial D_\gamma}{\partial d_{|\beta]}}\right)\right]+\frac{\rho}{T}r+\frac{1}{T}\frac{\partial f}{\partial \mathcal{E}_\mu}\alpha^{-1}_{\mu\alpha}j_\alpha\geq 0 \quad (20)$$

with $N_\alpha = \dot{d}_\alpha - d_\beta w_{\beta\alpha}$. Because the constitutive functions must not depend on the non objective quantity $w_{\beta\alpha} = \nabla_{[\alpha|}v_{|\beta]}$, the factor of $w_{\beta\alpha}$ vanishes. Exploitation of the residual inequality yields furthermore that the expressions in brackets at N_α, $\nabla_{(\alpha|}v_{|\beta)}$, $\nabla_\alpha\rho$, $\nabla_\alpha T$ respectively must vanish in equilibrium. These equilibrium conditions together with the Liu equation (14) are used to calculate the stress tensor

$$t_{\beta\alpha}=\frac{\partial f}{\partial B_\beta}B_\alpha+\mathcal{E}_\beta D_\alpha-(\nabla_\alpha d_\mu)\left(\frac{\partial f}{\partial\nabla_\beta d_\mu}-\mathcal{E}_\gamma\frac{\partial D_\gamma}{\partial\nabla_\beta d_\mu}\right)+$$
$$+\delta_{\alpha\beta}\left(-\rho^2\frac{\partial(f/\rho)}{\partial\rho}+\frac{\partial D_\mu}{\partial\rho}\mathcal{E}_\mu-\frac{\partial f}{\partial B_\gamma}B_\gamma-\mathcal{E}_\gamma D_\gamma\right) \quad (21)$$

and the surface couple density

$$2\,m_{\mu\beta\alpha}d_\mu=\frac{\partial f}{\partial\nabla_\alpha d_\beta}-\mathcal{E}_\mu\frac{\partial D_\mu}{\partial\nabla_\alpha d_\beta} \quad (22)$$

DIFFERENTIAL EQUATION FOR THE DIRECTOR FIELD

In equilibrium ($\dot{\underline{d}} = 0$, $\underline{\underline{l}} = 0$) the balance of moment of momentum assumes the form $\nabla_\gamma m_{\alpha\beta\gamma} + t_{[\alpha\beta]} = 0$, which together with the constitutive equatos (21) and (22) and the ansatz

$$f=+\frac{\varepsilon}{2}\mathcal{E}_\alpha\mathcal{E}_\alpha+\frac{\varepsilon_a}{2}(\mathcal{E}_\alpha d_\alpha)^2+\frac{K_1}{2}(\nabla_\alpha d_\beta)^2+\frac{K_2}{2}e_{\alpha\beta\gamma}d_\alpha(\nabla_\beta d_\gamma) \quad (23)$$

yields the following differential equation for the director field:

$$- \nabla_{\varphi} d_{[\alpha|} \left(K_1 \nabla_{\varphi} d_{|\beta]} + \frac{K_2}{2} e_{\mu\varphi|\beta]} d_{\mu} \right) - d_{[\alpha|} \left(\frac{K_2}{2} e_{\mu\varphi|\beta]} \nabla_{\varphi} d_{\mu} + \right.$$

$$\left. + K_1 \delta_{\mu\varphi} \delta_{\nu|\beta]} \nabla_{\varphi} \nabla_{\mu} d_{\nu} \right) + \mathcal{H}_{[\alpha|} B_{|\beta]} + \mathcal{E}_{[\alpha|} D_{|\beta]} +$$

$$+ \left(K_1 \nabla_{[\beta|} d_{\gamma} + \frac{K_2}{2} e_{\mu[\beta|\gamma} d_{\mu} \right) \nabla_{|\alpha]} d_{\gamma} = 0 \qquad (24)$$

Choosing the Ansatz for a distorted cholesteric helix:

$$\underline{d} = \left(\cos \varphi(z), \ \sin \varphi(z), \ 0 \right) \qquad (25)$$

results in the following differential equation ($\underline{\mathcal{E}} = (\mathcal{E},0,0)$):

$$0 = - K_1 \varphi' \varphi'' - \varepsilon_a \mathcal{E}^2 \cos \varphi \ \sin \varphi \ \varphi' \qquad (26)$$

which is the same one found by De Gennes from a variational principle of the free energy. Contrarily the present derivation is based on the second law of thermodynamics and the balance equations without assumptions on the minimality of the free energy in equilibrium.

RESULTS

The equations (18) and (19) for the dielectric displacement and the magnetic field have been extended to nonequilibrium. For a viscous heat conducting liquid crystal in electromagnetic fields in equilibrium the stress tensor and the surface density of couple have been calculated and a differential equation for the director field has been derived. In the case of a cholesteric helix in a homogeneous electric field with direction perpendicular to the helix axis this results in the differential equation derived by De Gennes[1].

The balance of momentum in equilibrium yields another differential equation, which together with equation (26) restricts the density dependence of the material constants[4].

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