The Equations of Motion for Nematics

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The fluid dynamics of nematics is discussed in terms of an approach based upon Rayleigh's dissipation function. In this way the derivation of the equations of motion becomes quite transparent.

1. Introduction

The fluid dynamics of nematics has been widely discussed. The most general derivation of the constitutive laws has been given by Hess [1]. His treatment contains both the Ericksen-Leslie-Parodi approach and the Harvard approach, which are extensively discussed in the review article by Stephen and Straley [2] and the book by de Gennes [3]. The purpose of this paper is to discuss the equations of motion for an anisotropic fluid from a slightly different point of view, namely starting from Rayleigh's dissipation function. Such an approach appears to be quite transparent.

Macroscopically the nematic fluid may be conceived as a continuous medium. The Eulerian description of fluid dynamics represents the state of an anisotropic fluid by a velocity field $\boldsymbol{v}(\boldsymbol{r}, t)$, a pressure field $p(\boldsymbol{r}, t)$, a density field $\varrho(\boldsymbol{r}, t)$, an inertial tensor field $\mathbf{I}(\boldsymbol{r}, t)$ and a tensor order parameter field $\mathbf{Q}(\boldsymbol{r}, t)$. Because of the local uniaxiality of the medium the tensor elements $I_{\alpha\beta}$ and $Q_{\alpha\beta}$, which are due to the anisotropy, are given by

$$I_{\alpha\beta} = I_{\perp}\,\delta_{\alpha\beta} + (I_{\parallel} - I_{\perp})\,n_\alpha n_\beta\,, \tag{1.1}$$

$$Q_{\alpha\beta} = S\,(n_\alpha n_\beta - \tfrac{1}{3}\,\delta_{\alpha\beta})\,, \tag{1.2}$$

where S denotes the order parameter of the nematic and n_α is the α-th component of the local director $\boldsymbol{n}(\boldsymbol{r}, t)$.

For reasons of simplicity the fluid is assumed to be incompressible, i.e. the density field $\varrho(\boldsymbol{r}, t)$ is constant, $\varrho(\boldsymbol{r}, t) = \varrho$, and $\partial_\alpha v_\alpha = 0$; repeated indices must be summed, $\alpha = x, y, z$. Viscous fluids are described by the Navier-Stokes equation

$$\varrho\,\partial_t v_\alpha = -\,\partial_\beta\,(\Pi_{\beta\alpha} - \sigma_{\beta\alpha})\,, \tag{1.3}$$

with $\Pi_{\alpha\beta}$ denoting the momentum flux density tensor defined by

$$\Pi_{\alpha\beta} = p\,\delta_{\alpha\beta} + \varrho\,v_\alpha v_\beta\,, \tag{1.4}$$

where the contribution of the elastic distortion is neglected because of its smallness, and $\sigma_{\alpha\beta}$ the viscosity stress tensor, which can be obtained from Rayleigh's dissipation function D by means of

$$\sigma_{\alpha\beta} = \frac{\partial D}{\partial\,\partial_\alpha v_\beta}\,. \tag{1.5}$$

The Navier-Stokes equation alone does not suffice because of the coupling between the flow and the rotational motion of the anisotropy. Consequently equations of motion are needed to describe the time-dependent behaviour of the anisotropy. This means, putting

$$n_x = \sin\theta(\boldsymbol{r}, t)\cos\varphi(\boldsymbol{r}, t),$$
$$n_y = \sin\theta(\boldsymbol{r}, t)\sin\varphi(\boldsymbol{r}, t),$$
$$n_z = \cos\theta(\boldsymbol{r}, t) \tag{1.6}$$

that the equations of motion for the functions $\varphi(\boldsymbol{r}, t)$ and $\theta(\boldsymbol{r}, t)$ are required. The kinetic energy of the rotating anisotropy is given by

$$T = \tfrac{1}{2}\,I_{\alpha\beta}\,\omega_\alpha\,\omega_\beta\,, \tag{1.7}$$

where $\boldsymbol{\omega}$ denotes the angular velocity of the rotating anisotropy, or using the representation of $\boldsymbol{\omega}$ in Eulerian angles and neglecting the "spin" of the rotating anisotropy

$$T = \tfrac{1}{2}\,I_{\perp}(\dot\varphi^2\sin^2\theta + \dot\theta^2) + \tfrac{1}{2}\,I_{\parallel}\,\dot\varphi^2\cos^2\theta\,. \tag{1.8}$$

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Now the equations of motion read according to Lagrange

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot\theta}\right)-\frac{\partial T}{\partial \theta}=-\frac{\partial D}{\partial \dot\theta}-\frac{\partial F_{\mathrm{el}}}{\partial \theta}, \tag{1.9 a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot\varphi}\right)=-\frac{\partial D}{\partial \dot\varphi}-\frac{\partial F_{\mathrm{el}}}{\partial \varphi} \tag{1.9 b}$$

where $\partial D/\partial\dot\theta$ and $\partial D/\partial\dot\varphi$ are generalized frictional forces and $\partial F_{\mathrm{el}}/\partial\theta$ and $\partial F_{\mathrm{el}}/\partial\varphi$ generalized elastic forces, which arise because of the elastic distortion of the medium. The quantity F_{el} denotes the well-known Frank distortion free energy density [4]

$$F_{\mathrm{el}}=\tfrac{1}{2}K_1(\operatorname{div}\boldsymbol{n})^2+\tfrac{1}{2}K_2(\boldsymbol{n}\cdot\operatorname{rot}\boldsymbol{n})^2+\tfrac{1}{2}K_3(\boldsymbol{n}\times\operatorname{rot}\boldsymbol{n})^2, \tag{1.10}$$

where K_1, K_2 and K_3 are the elastic constants for splay, twist and bend respectively.

Clearly then the equations of motion are known as soon as Rayleigh's dissipation function D is known.

2. Rayleigh's Dissipation Function

The relevant quantities to construct Rayleigh's dissipation function are the tensors $\partial_\alpha v_\beta$, $Q_{\alpha\beta}$ and $\dot Q_{\alpha\beta}$. Instead of $Q_{\alpha\beta}$ and $\dot Q_{\alpha\beta}$, however, the simpler tensors $n_\alpha n_\beta$ and $\dot n_\alpha n_\beta$ may be taken. Rayleigh's dissipation function D consists now of all possible invariants, which can be constructed from these tensors, but these invariants must be bilinear in the tensors $\partial_\alpha v_\beta$ and $\dot n_\alpha n_\beta$. It follows directly that, in case of an anisotropic incompressible fluid, the general expression for Rayleigh's dissipation function is given by

$$\begin{aligned}D=&\tfrac{1}{2}\eta\,\partial_\alpha v_\beta\partial_\alpha v_\beta+\tfrac{1}{2}\xi\,\partial_\alpha v_\beta\partial_\beta v_\alpha\\&+\tfrac{1}{2}\xi_1 n_\alpha n_\beta\partial_\alpha v_\gamma\partial_\beta v_\gamma+\tfrac{1}{2}\xi_2 n_\alpha n_\beta\partial_\gamma v_\alpha\partial_\gamma v_\beta\\&+\xi_3 n_\alpha n_\beta\partial_\gamma v_\alpha\partial_\beta v_\gamma+\tfrac{1}{2}\xi_4 n_\alpha n_\beta n_\gamma n_\delta\partial_\alpha v_\beta\partial_\gamma v_\delta\\&+\xi_5\dot n_\alpha n_\beta\partial_\beta v_\alpha+\xi_6\dot n_\alpha n_\beta\partial_\alpha v_\beta+\tfrac{1}{2}\xi_7\dot n_\alpha\dot n_\alpha.\end{aligned} \tag{2.1}$$

Then the viscosity stress tensor $\sigma_{\alpha\beta}$ reads

$$\begin{aligned}\sigma_{\alpha\beta}=&\eta\,\partial_\alpha v_\beta+\xi\,\partial_\beta v_\alpha+\xi_1 n_\alpha n_\gamma\partial_\gamma v_\beta+\xi_2 n_\beta n_\gamma\partial_\alpha v_\gamma\\&+\xi_3 n_\beta n_\gamma\partial_\gamma v_\alpha+\xi_3 n_\alpha n_\gamma\partial_\beta v_\gamma\\&+\xi_4 n_\alpha n_\beta n_\gamma n_\delta\partial_\gamma v_\delta+\xi_5\dot n_\beta n_\alpha+\xi_6\dot n_\alpha n_\beta.\end{aligned} \tag{2.2}$$

The appearing coefficients are not all independent, because D and $\sigma_{\alpha\beta}$ must vanish, when the whole fluid is in uniform rotation, i.e. when

$$\partial_\beta v_\alpha=\varepsilon_{\alpha\mu\beta}\,\omega_\mu,\quad \dot n_\alpha=\varepsilon_{\alpha\mu\beta}\,\omega_\mu\,n_\beta, \tag{2.3 a, b}$$

where ω_μ is the μ-th component of the angular velocity $\boldsymbol{\omega}$ and $\varepsilon_{\alpha\beta\gamma}$ is the Levi-Civita tensor, which is defined as

$$\varepsilon_{\alpha\beta\gamma}=\begin{cases}1, & \text{if}\ \ \alpha\beta\gamma=xyz, yzx, zxy,\\ -1, & \text{if}\ \ \alpha\beta\gamma=zyx, yxz, xzy\\ 0, & \text{otherwise.}\end{cases}$$

Substitution of (2.3) into (2.1) and (2.2) gives

$$\begin{aligned}D=&(\eta-\xi)\,\omega_\alpha\omega_\alpha+(\tfrac{1}{2}\xi_1+\tfrac{1}{2}\xi_2-\xi_3+\xi_5-\xi_6+\tfrac{1}{2}\xi_7)\\&\cdot(\omega_\alpha\omega_\alpha-n_\alpha n_\beta\,\omega_\alpha\omega_\beta)=0,\end{aligned} \tag{2.4 a}$$

$$\begin{aligned}\sigma_{\alpha\beta}=&(\eta-\xi)\,\varepsilon_{\beta\mu\alpha}\,\omega_\mu+(\xi_1-\xi_3-\xi_5)\,\varepsilon_{\beta\mu\gamma}\,n_\alpha n_\gamma\,\omega_\mu\\&+(\xi_2-\xi_3-\xi_6)\,\varepsilon_{\gamma\mu\alpha}\,n_\beta n_\gamma\,\omega_\mu=0.\end{aligned} \tag{2.4 b}$$

The Eq. (2.4) imply immediately

$$\eta-\xi=0, \tag{2.5 a}$$

$$\xi_5=-\xi_1+\xi_3, \tag{2.5 b}$$

$$\xi_6=\xi_2-\xi_3, \tag{2.5 c}$$

$$\xi_7=\xi_1+\xi_2-2\xi_3, \tag{2.5 d}$$

i.e. only five independent coefficients of viscosity appear.

Concluding Rayleigh's dissipation function for an incompressible anisotropic fluid reads

$$\begin{aligned}D=&\tfrac{1}{2}\eta(\partial_\alpha v_\beta\partial_\alpha v_\beta+\partial_\alpha v_\beta\partial_\beta v_\alpha)\\&+\tfrac{1}{2}\xi_1(n_\alpha\partial_\alpha v_\gamma-\dot n_\gamma)(n_\beta\partial_\beta v_\gamma-\dot n_\gamma)\\&+\tfrac{1}{2}\xi_2(n_\alpha\partial_\gamma v_\alpha+\dot n_\gamma)(n_\beta\partial_\gamma v_\beta+\dot n_\gamma)\\&+\xi_3(n_\alpha\partial_\alpha v_\gamma-\dot n_\gamma)(n_\beta\partial_\gamma v_\beta+\dot n_\gamma)\\&+\tfrac{1}{2}\xi_4 n_\alpha n_\beta n_\gamma n_\delta\partial_\alpha v_\beta\partial_\gamma v_\delta,\end{aligned} \tag{2.6}$$

whereas the associated viscosity stress tensor is given by

$$\begin{aligned}\sigma_{\alpha\beta}=&\eta(\partial_\alpha v_\beta+\partial_\beta v_\alpha)+\xi_1 n_\alpha(n_\gamma\partial_\gamma v_\beta-\dot n_\beta)\\&+\xi_2 n_\beta(n_\gamma\partial_\alpha v_\gamma+\dot n_\alpha)+\xi_3 n_\beta(n_\gamma\partial_\gamma v_\alpha-\dot n_\alpha)\\&+\xi_3 n_\alpha(n_\gamma\partial_\beta v_\gamma+\dot n_\beta)+\xi_4 n_\alpha n_\beta n_\gamma n_\delta\partial_\gamma v_\delta.\end{aligned} \tag{2.7}$$

The viscosity coefficients appearing in (2.7) can be easily expressed in the Leslie coefficients α_i ($i=1,2,\ldots,6$) by comparing the expression (2.7) with the Leslie viscosity tensor [5]

$$\sigma_{\alpha\beta} = \tfrac{1}{2}\alpha_4(\partial_\alpha v_\beta + \partial_\beta v_\alpha) + \tfrac{1}{2}(\alpha_5 - \alpha_2)\, n_\alpha n_\gamma \partial_\gamma v_\beta + \tfrac{1}{2}(\alpha_6 + \alpha_3)\, n_\beta n_\gamma \partial_\alpha v_\gamma + \tfrac{1}{2}(\alpha_6 - \alpha_3)\, n_\beta n_\gamma \partial_\gamma v_\alpha + \tfrac{1}{2}(\alpha_5 + \alpha_2)\, n_\alpha n_\gamma \partial_\beta v_\gamma + \alpha_2 n_\alpha \dot n_\beta + \alpha_3 n_\beta \dot n_\alpha + \alpha_1 n_\alpha n_\beta n_\gamma n_\delta \partial_\gamma v_\delta . \tag{2.8}$$

Then it is found that

$$\xi_1 = \tfrac{1}{2}(\alpha_5 - \alpha_2), \tag{2.9a}$$

$$\xi_2 = \tfrac{1}{2}(\alpha_6 + \alpha_3), \tag{2.9b}$$

$$\xi_3 = \tfrac{1}{2}(\alpha_6 - \alpha_3) = \tfrac{1}{2}(\alpha_5 + \alpha_2), \tag{2.9c}$$

$$\xi_4 = \alpha_1, \tag{2.9d}$$

$$\eta = \tfrac{1}{2}\alpha_4 . \tag{2.9e}$$

It follows directly that Leslie's original assumption of six independent viscosity coefficients does not hold because of the Parodi-relation [6]

$$\alpha_6 - \alpha_3 = \alpha_5 + \alpha_2 . \tag{2.10}$$

The number of viscosity coefficients is reduced from six to five, because not only the viscosity tensor $\sigma_{\alpha\beta}$ must vanish when the whole fluid is in uniform rotation but the dissipation energy as well. The last requirement reduces the number of viscosity coefficients from six to five.

It should be remarked here that the coefficients η, ξ_1 and ξ_2 are closely related with the three principle viscosity coefficients introduced by Miesowicz [7]. Using the notation of Helfrich [8] it appears that

$$\eta_1 = \eta + \xi_1 , \tag{2.11a}$$

$$\eta_2 = \eta + \xi_2 , \tag{2.11b}$$

$$\eta_3 = \eta . \tag{2.11c}$$

The generalized frictional forces are given by

$$\frac{\partial D}{\partial \dot\theta} = [(\xi_1 + \xi_2 - 2\xi_3)\, \dot n_\gamma - (\xi_1 - \xi_3)\, n_\alpha \partial_\alpha v_\gamma + (\xi_2 - \xi_3)\, n_\alpha \partial_\gamma v_\alpha] \frac{\partial \dot n_\gamma}{\partial \dot\theta}, \tag{2.12a}$$

$$\frac{\partial D}{\partial \dot\varphi} = [(\xi_1 + \xi_2 - 2\xi_3)\, \dot n_\gamma - (\xi_1 - \xi_3)\, n_\alpha \partial_\alpha v_\gamma + (\xi_2 - \xi_3)\, n_\alpha \partial_\gamma v_\alpha] \frac{\partial \dot n_\gamma}{\partial \dot\varphi}. \tag{2.12b}$$

Usually the appearing combinations of ξ coefficients are rewritten in terms of the coeffients γ_1 and γ_2 defined by

$$\gamma_1 = \xi_1 + \xi_2 - 2\xi_3 , \tag{2.13a}$$

$$\gamma_2 = \xi_2 - \xi_1 . \tag{2.13b}$$

It can be easily checked that the generalized frictional forces vanish when the whole fluid is in uniform rotation.

Finally three remarks should be made in view of existing approaches. First of all the present approach directly relates to the experimentally observable Miesowicz viscosities. Secondly the fact that the director is a unit vector is directly taken ito account. In this way the introduction of the so-called "molecular field", which has no physical origin at all, is rightly avoided. The third remark concerns Rayleigh's dissipation function. This function is nothing but half the dissipation energy density, i.e. integration of this function over the volume of the system results into half the energy dissipation $T\dot S$ in an isothermal process.

Note added in proof: During the fifth liquid crystal conference of socialist countries (Odessa, USSR, October 1983) Dr. B. Ya. Zeldovich brought to my notice a preliminary version of his recent work showing quite clearly that he arrived, quite independently, at the same conclusion, i.e. the Parodi relation can be derived from Rayleigh's dissipation function.

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