Remarks on the flow alignment of disc like nematics

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Résumé. — Dans le cadre de la théorie hydrodynamique de Leslie, Ericksen et Parodi, on examine la nature de l'orientation des cristaux liquides nématiques dans une expérience d'écoulement. On montre que l'alignement ne peut se produire que dans un intervalle d'angle limité. L'application au cas des nématiques discotiques montre que seule l'une des deux théories récemment discutées sur l'origine de l'alignement d'écoulement [2-4] est en bon accord avec la théorie de l'hydrodynamique des nématiques.

Abstract. — The nature of the flow alignment of nematic liquid crystals is discussed within the hydrodynamic theory of Leslie, Ericksen and Parodi. It is shown that there is a limited range of angles for which flow alignment can occur. With this as a starting point the flow alignment of disc like nematics is discussed. It is proved that only one out of the two models of flow alignment recently discussed in the literature [2-4] is consistent with the hydrodynamic theory of nematics.

1. Introduction.

Since the existence of discotic liquid crystals was first reported by Chandrasekhar et al. [1] there have appeared an increasing number of papers, both theoretical and experimental, concerning these systems. Although there have been no papers reporting an experimental study of the flow properties of the discotics (at least to the knowledge of this author) two theoretical papers have recently appeared [2-4], concerning flow alignment of nematic discotics under shear. The flow alignment predicted by Carlsson [2] is shown in figure 1a and the prediction by Brand and Pleiner [3] is shown in figure 1b. In an erratum to their paper [4] Brand and Pleiner however modify their prediction to be consistent with that of figure 1a. It is the aim of this paper to show that it is only the situation pictured in figure 1a that is consistent with the hydrodynamic theory of nematic liquid crystals developed by Leslie, Ericksen and Parodi (the LEP-theory). It is also shown that although the flow alignment pictured in figure 1b represents an equilibrium solution of the hydrodynamic equations, this solution is not physically feasible, because it describes an equilibrium which is unstable, so a system with this configuration would relax to the situation pictured in figure 1a due to fluctuations.

Fig. 1. — Predictions of the flow alignment of nematic discotics which have been discussed in the literature [2-4]. We show in this paper that figure 1a represents a stable equilibrium while figure 1b represents an unstable one.
2. Flow alignment.

In this section we discuss the flow alignment of nematics in the spirit of the LEP-Theory. The results displayed below were originally discussed by Ericksen [5] and recently reviewed by Leslie [6]. We introduce coordinates as shown in figure 2. We study a nematic under shear. The nematic is confined between two parallel glass plates, the upper plate moving in the x-direction with a velocity v. Assuming the director (denoted by \( \hat{n} \)) to remain in the plane of shear we introduce a coordinate \( \theta \) to describe it, where \( \theta \) is the angle between the director and the normal to the glass plates and is counted as positive for a clockwise rotation. At the present stage we have not restricted ourselves to the study of either rod-like or disc-like nematics. The meaning of the director in these two different cases is shown in figure 2. The equivalence of \( \hat{n} \) with \( -\hat{n} \) allows us to study \( \theta \) only in the interval \( [ -90^\circ, 90^\circ] \).

![Fig. 2. Definition of coordinates in the present work.](image)

When we study flow alignment we must consider two of the six Leslie viscosities, \( \alpha_2 \) and \( \alpha_3 \). It is important to notice the following inequality [7] which must be fulfilled by these:

\[
\alpha_3 - \alpha_2 \geq 0. \tag{1}
\]

The viscous torque, \( \Gamma^p_z \), exerted on the director in the stationary state (i.e. \( \partial \theta / \partial t = 0 \)) is given by

\[
\Gamma^p_z = (\alpha_3 \sin^2 \theta - \alpha_2 \cos^2 \theta) u' \tag{2}
\]

where \( u' \) is the local shear. Flow alignment is possible when \( \Gamma^p_z \) is zero giving the following solution for the flow alignment angle \( \theta_n \):

\[
\tan \theta_n = \pm \sqrt{\alpha_2 / \alpha_3}. \tag{3}
\]

We can divide the solutions of equation (3) into two different cases. Either both \( \alpha_2 \) and \( \alpha_3 \) are negative (case a) or both are positive (case b). The two signs in the solution of equation (3) represents one stable and one unstable solution. It is easy to show (see for instance Ref. [2]) that when \( \alpha_2 \) and \( \alpha_3 \) are negative it is the + sign which gives the stable solution. When \( \alpha_2 \) and \( \alpha_3 \) are positive however it is the − sign which has to be chosen to give the stable solution.

**Case a : \( \alpha_2 \) and \( \alpha_3 \) are negative.** — In this case the inequality (1) implies that \( |\alpha_2| \geq |\alpha_3| \). As is mentioned earlier the stable solution of equation (3) is the one given by the + sign. This means that the allowed values of \( \tan \theta_n \) will be in the interval \([1, \infty[\) and we thus get:

\[
\theta_n \in [45^\circ, 90^\circ]. \tag{4}
\]

**Case b : \( \alpha_2 \) and \( \alpha_3 \) are positive.** — In this case the inequality (1) implies that \( \alpha_3 \geq \alpha_2 \). The stable solution of equation (3) is now given by the − sign. The allowed values of \( \tan \theta_n \) will now be in the interval \([ -1, 0[\) and we thus get:

\[
\theta_n \in [ -45^\circ, 0^\circ]. \tag{5}
\]

We thus draw the conclusion that flow alignment is possible either with a value of \( \theta_n \) between \( -45^\circ \) and \( 0^\circ \) (when \( \alpha_2 \) and \( \alpha_3 \) are both positive) or between \( 45^\circ \) and \( 90^\circ \) (when \( \alpha_2 \) and \( \alpha_3 \) are both negative). This is illustrated in figure 3.

![Fig. 3. Possible values of the flow alignment angle within the LEP-theory (shaded areas). A flow alignment angle between \(-45^\circ\) and \(0^\circ\) is consistent with positive values of \(\alpha_2\) and \(\alpha_3\), while a flow alignment angle between \(45^\circ\) and \(90^\circ\) is consistent with negative values of \(\alpha_2\) and \(\alpha_3\). The areas not shaded in the figure represent the unstable solutions of equation (3) and are not physically feasible. The definition of \(\theta\) is shown in the upper left part of the figure.](image)


Recently two papers have appeared predicting the nature of flow alignment of disc-like nematics. The predictions given in these two papers are illustrated in figure 1. By the aid of the discussion in section 2 (the results are summarized in Fig. 3), we immediately see that the situation pictured in figure 1b represents an unstable equilibrium while that of figure 1a represents a stable one. We also see that disc-like nematics
demand positive values of the Leslie viscosities $a_2$ and $a_3$ (in the case where flow alignment occurs). The reasoning which led to the proposal of figure 1a was based on a calculation by Volovic [8], and is discussed in reference [2]. Here we will however mention a calculation of the flow alignment angle for uniaxial nematics by Forster [9] and show that the prediction of figure 1a is consistent also with this. With the choice of $\theta$ made in this work, the calculations by Forster establish that the flow alignment angle is given by

$$\tan^2 \theta_n = \frac{I_1 + 2 I_2 + 2 S(I_1 - I_2)}{I_1 + 2 I_2 - S(I_1 - I_2)}$$

(6)

$S$ is the order parameter of the system and $I_2$ and $I_3$ are the components of the molecular moments of inertia evaluated in the system of principal molecular axes as defined by Forster. We can distinguish two special types of molecules: rod-like molecules where $I_1 \to 0$ and disc-like molecules where $I_1 \to 0$.

**Rod-like molecules** ($I_1 = 0$). -- Putting $I_1 = 0$ in equation (6) we get

$$\tan^2 \theta_n = \frac{1}{1 - S}.$$  

(7)

By letting $S$ increase from 0 to 1 we see that $\tan^2 \theta_n$ lies in to the interval $[1, \infty]$. This corresponds to case a mentioned in section 2 and rod-like nematics should be described by negative values of $a_2$ and $a_3$ and have a flow alignment angle $\theta_n$ which lies between $-45^\circ$ and $0^\circ$ depending on the order parameter. For values of $S$ close to one, $\theta_n$ is small and negative which implies $a_3 \gg a_2$ according to equations (3) and (8). (We only discuss discotics showing flow alignment and do not pay attention to the possibility of tumbling, which resembles the situation that occurs for some of rod-like nematics.)

**Disc-like molecules** ($I_1 = 0$). -- If we put $I_1 = 0$ in equation (6) we get

$$\tan^2 \theta_n = \frac{2(1 - S)}{2 + S}.$$  

(8)

By letting $S$ increase from 0 to 1 we see that $\tan^2 \theta_n$ lies in the interval $[1, 0]$. This is case b discussed in section 2. Disc-like nematics therefore should be described by positive values of $a_2$ and $a_3$ and the flow alignment angle should lie between $-45^\circ$ and $0^\circ$ depending on the order parameter. For values of $S$ close to one, $\theta_n$ is small and negative which implies $a_2 \gg a_3$ according to equations (3) and (8). (We only discuss discotics showing flow alignment and do not pay attention to the possibility of tumbling, which resembles the situation that occurs for some of rod-like nematics.)


Two models of the nature of flow alignment of disc-like nematics have recently been discussed in the literature [2-4]. We have shown that the model suggested in figure 1a represents a stable equilibrium while that of figure 1b represents an unstable one. We have also shown (as far as flow alignment is concerned) that as a consequence of Forster's calculations [9] rod-like nematics must be described by negative values of $a_2$ and $a_3$ while the disc-like nematics must be assigned positive values of both these constants. This is in accordance with the earlier predictions by Carlsson [2].

In figure 4 we have shown the flow alignment of disc-like and rod-like nematics, and we see that the physical situations in the two cases are quite similar. In figure 4a we have rods lying almost parallel to the flow direction while in figure 4b we have discs which are oriented with the disc planes almost parallel to the same direction (this is the situation occurring for a value of the order parameter which is not very much less than one). The similarity of the two cases should not be surprising if one imagines some kind of steric force to be responsible for the flow alignment.

![Flow alignment diagram](image)

**Fig. 4.** -- Flow alignment angle, $\tan \theta_n = \sqrt{a_2/a_3}$, for rod-like molecules. Both $a_2$ and $a_3$ are negative and $|a_2| \gg |a_3|$ (left). Proposed flow alignment angle, $\tan \theta_n = -\sqrt{a_2/a_3}$, for disc like molecules. Both $a_2$ and $a_3$ are positive and $a_3 \gg a_2$ (right).

References