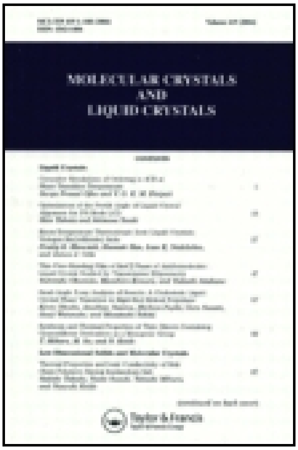

Molecular Crystals and Liquid Crystals

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl20

Effect of a Hydrodynamic Flow on the Orientation Profiles of a Nematic Liquid Crystal Around a Spherical Particle

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Version of record first published: 31 Aug 2006

Mol. Cryst. Liq. Cryst., Vol. 435, pp. 75/[735]–85/[745], 2005

ISSN: 1542-1406 print/1563-5287 online
DOI: 10.1080/15421400590956009

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We study the effect of a hydrodynamic flow on the orientational configuration of a nematic liquid crystal around a spherical particle imposing rigid normal anchoring. We discuss the cases of large Ericksen numbers (characterizing the ratio of viscous force to the elastic force), where strong elastic deformation by the flow is expected. We assume the Stokes flow profile and deal with a simplified dynamic equation of the orientational order parameter of a second-rank tensor $Q_{\alpha\beta}$. We consider the cases where a particle accompanying a hyperbolic hedgehog or a Saturn ring is subjected to a flow along the axis of rotational symmetry. In both cases the orientation profiles exhibit considerable deformation by a flow.

Keywords: colloid; hydrodynamic flow; hyperbolic hedgehog; nematic liquid crystal; Saturn ring; tensor order parameter

I. INTRODUCTION

Liquid crystal colloidal dispersions [1–7] provide a novel class of composite materials that show structures and mechanical properties different from conventional colloidal systems. They have therefore

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been attracting considerable interest in technology as well as in fundamental science. The elastic distortions of the host liquid crystal due to the surface anchoring of particles or droplets immersed in it bring about various interesting properties unique to liquid crystal colloidal dispersions. For instance, such elastic distortions can mediate long-range interaction between particles, yielding a rich variety of superstructures formed by immersed particles, including linear chains [2,3,6], anisotropic clusters [1], and periodic lattices [7].

Another interesting feature of liquid crystal colloidal dispersions is that immersed particles can be accompanied by topological defects to preserve the neutrality of topological charges when the surface anchoring of the particles and the resultant elastic distortions of the host liquid crystal are strong enough. In the case of a nematic liquid crystal as a host fluid, experimentally observed topological defects include a point-like defect referred to as a hyperbolic hedgehog [2,3], a Saturn ring that encircles a particle as the name implies [8], and two surface defects located at the poles of a particle known as boojums [3]. Topological defects arising in liquid crystals in response to foreign inclusions provide an interesting problem on its own, because topological defects have long been one of the important subjects of condensed matter physics. In particular, liquid crystals have been extensively studied as one of the experimentally accessible systems showing a rich variety of topological defects depending on the symmetry of liquid crystal phases. Moreover, it has been known that the interaction between particles and the resultant superstructures sensitively depends on what kind of topological defects accompany the particles.

In this article we focus on the dynamical aspects of the orientation profiles and the topological defects in a nematic liquid crystal around a spherical particle when a hydrodynamic flow is imposed as an external perturbation. There have been experimental [9] and numerical [10–12] studies concerning the effect of other types of external perturbations: an electric or magnetic field. It has been shown that when an electric or magnetic field parallel to the axis of rotational symmetry is applied to the hedgehog configuration, it becomes unstable to transform itself into a Saturn ring. The effect of a hydrodynamic flow is less well understood. Many of the previous studies [13–15] concerning a nematic liquid crystal around a particle under flow considered fixed orientation profiles under strong external aligning fields or in the cases with weak flows (to be more precise, with small Ericksen numbers characterizing the ratio of viscous force to the elastic force of a nematic liquid crystal). The change in the orientation profiles under a strong flow was investigated by Stark and Ventzki [16], who solved the Ericksen-Leslie equation for the director field $\boldsymbol{n}$ to find stationary profiles of the orientational order around a spherical particle under flow. They showed that the motion of a hyperbolic hedgehog is against the flow direction, in striking contrast to an intuitive argument that a defect may be convected by the flow. However, an interesting problem whether a hydrodynamic flow can induce structural transition of a topological defect remains open, because the treatment of the orientational order in terms of $\boldsymbol{n}$ inevitably suffers from singularities at the topological defects.

In the present article to avoid the singularities from topological defects, we employ a second-rank tensor order parameter $Q_{\alpha\beta}$ for the description of the orientational order of a nematic liquid crystal. As a first step towards the understanding of the motion of topological defects, we make a simplifying assumption that the flow profile is that of a Stokes flow. Then we do not have to solve the equation for the fluid velocity and we only have to deal with the equation of motion for $Q_{\alpha\beta}$. We can employ straightforwardly an adaptive mesh refinement scheme developed previously [11,12,17,18] for the investigation of an equilibrium fine structure of topological defects and their dynamical behavior under an applied magnetic or electric field. We discuss the cases where a spherical particle with rigid normal surface anchoring accompanied by a hyperbolic hedgehog or a Saturn ring is exposed to a flow along the axis of rotational symmetry.

II. MODEL

We consider a spherical particle of radius R_0 with rigid normal surface anchoring whose center is fixed and located at the origin of the coordinate system. The orientational order at infinity is taken to be uniform and parallel to the z-axis. At infinity, a uniform flow is imposed along the z-axis (parallel to the orientational order) with speed v_∞. At the particle surface, a no-slip boundary condition is employed, so that $\boldsymbol{v} = 0$ there.

As noted in the Introduction, we use a second-rank traceless tensor order parameter $Q_{\alpha\beta}$ for the description of the orientational order of a nematic liquid crystal. It enables one to deal with topological defects without introducing any singularities. There have been several theoretical attempts [19,20] to formulate the hydrodynamic equations for $Q_{\alpha\beta}$ and the velocity field $\boldsymbol{v}$. We begin with those given by Olmsted and Goldbart [19]. After some appropriate rescaling of the length, the time, and the order parameter $Q_{\alpha\beta}$, they are written as

$$Re\left(\frac{\partial}{\partial t} + \boldsymbol{v}\cdot\nabla\right)v_\alpha = \partial_\gamma\left[2V^{[s]}_{\gamma\alpha} + \frac{1}{Er^*}\left(-\bar{\beta}_1 H^{[s]}_{\gamma\alpha} + \sigma^{i[a]}_{\gamma\alpha} + \sigma^{d}_{\gamma\alpha}\right) - p\delta_{\gamma\alpha}\right], \quad [1]$$

$$\left(\frac{\partial}{\partial t}+\boldsymbol{v}\cdot\boldsymbol{\nabla}\right)\boldsymbol{Q}_{\alpha\beta}-(V^{[a]}_{\alpha\gamma}\boldsymbol{Q}_{\gamma\beta}-\boldsymbol{Q}_{\alpha\gamma}V^{[a]}_{\gamma\beta})=\bar{\beta}_1V^{[s]}_{\alpha\beta}+\frac{1}{\bar{\beta}_2Er^*}H^{[s]}_{\alpha\beta}. \qquad (2)$$

Here the length and the time are given in units of R_0 and R_0/v_∞, respectively. The velocity gradient tensor is defined as $V_{\alpha\beta}=\partial_\beta v_\alpha$. The superscripts $[s]$ and $[a]$ denote the symmetric and the anti-symmetric components of a second-rank tensor, respectively. The precise form of the molecular field $H_{\alpha\beta}\equiv-\delta F/\delta \boldsymbol{Q}_{\alpha\beta}$ after rescaling will be given below (F is the free energy of the system). $\sigma^{i[a]}_{\alpha\beta}=H^{[s]}_{\alpha\gamma}\boldsymbol{Q}_{\gamma\beta}-\boldsymbol{Q}_{\alpha\gamma}H^{[s]}_{\gamma\beta}$ is the anti-symmetric component of the stress tensor arising from the coupling between the orientational order and the flow. The elastic stress is given by $\sigma^d_{\alpha\beta}=-(\partial F/\partial(\partial_\alpha \boldsymbol{Q}_{\mu\nu}))\partial_\beta \boldsymbol{Q}_{\mu\nu}$. The rescaled kinetic coefficient $\bar{\beta}_1$ is associated with the off-diagonal kinetic coupling between $\boldsymbol{Q}_{\alpha\beta}$ and $\boldsymbol{v}$. Another kinetic coefficient $\bar{\beta}_2$ is the rescaled rotational viscosity.

After the rescaling, the molecular field $H_{\alpha\beta}$ reads

$$H_{\alpha\beta}=-\tau\boldsymbol{Q}_{\alpha\beta}+\frac{3\sqrt{6}}{4}\boldsymbol{Q}_{\alpha\gamma}\boldsymbol{Q}_{\gamma\beta}-(Tr\boldsymbol{Q}^2)\boldsymbol{Q}_{\alpha\beta}+{\xi_R}^2\nabla^2\boldsymbol{Q}_{\alpha\beta}. \qquad (3)$$

The dimensionless nematic coherence length is defined as $\xi_R\equiv\sqrt{L_1/Cs^2}/R_0$, with $s\equiv 2\sqrt{6}|B|/9C$ (see footnote [21] for the definitions of B, C, and L_1).

One of the important dimensionless quantities characterizing the problem is the ratio of viscous force to the elastic force of a nematic liquid crystal:

$$Er=\frac{Er^*}{{\xi_R}^2}=\frac{\beta_3 v_\infty R_0}{2s^2L_1}, \qquad (4)$$

where β_3 is associated with the isotropic part of the viscosity whose precise definition can be found in Reference [19]. Er is nothing more than the Ericksen number apart from the numerical factor. The Reynolds number $Re=2\rho v_\infty R_0/\beta_3$, with ρ being the mass density of the liquid crystal, is much smaller than unity in the present problems.

Here we make a simplifying assumption; the flow profile is given by that of a Stokes flow [22]. We notice here that in Eq. (1) the anisotropy of the viscosity is not taken into account. One might naively think that in the case of isotropic viscosity, such an assumption is justified for large Ericksen number limit. However this may not be the case because from Eq. (2) the molecular field can be of the order of Er^*. Here we adopt the assumption of Stokes flow for practical reasons; to solve Eqs. (1) and (2) strictly, the determination of the flow profile $\boldsymbol{v}$ for a given profile of the order parameter $\boldsymbol{Q}_{\alpha\beta}$ is necessary at each iteration for the update of $\boldsymbol{Q}_{\alpha\beta}$ and it is highly demanding computationally. When the flow profile is assumed and fixed, the numerical resources required for calculating the time evolution of $Q_{\alpha\beta}$ is greatly reduced. The numerical results here are presented just as a first trial for the investigation of the motion of a topological defect accompanying a particle.

The numerical implementation for solving the equation of motion for $Q_{\alpha\beta}$ is the same as that prescribed in detail in Ref. [18], where rotational symmetry about the z-axis is assumed and an adaptive mesh refinement scheme is employed to deal with topological defects whose core dimensions are much smaller than that of a particle. The parameters chosen are $\bar{\beta}_1 = 1.4$, $\bar{\beta}_2 = 2$, and $\xi_R = 5 \times 10^{-3}$. The reduced temperature is set to $\tau = (3\sqrt{6} - 8)/12$ so that an order parameter with uniaxial symmetry $Q_{\alpha\beta} = Q_0(n_\alpha n_\beta - (1/3)\delta_{\alpha\beta})$ with $Q_0 = 1$ minimizes the bulk energy (here $\boldsymbol{n}$ is an arbitrary unit vector corresponding to the director). Since we are interested in the situation where the effect of the fluid flow and the resultant elastic distortion of the liquid crystal are strong enough, we choose $Er = 10$. We start our numerical calculations with the equilibrium hedgehog or Saturn-ring profile without flow.

III. RESULTS

We first show our results with a hyperbolic hedgehog profile as the initial condition. Figure 1 presents the time evolution of the orientation profile from a hedgehog configuration under a hydrodynamic flow whose direction is from the hedgehog to the particle. The orientation profiles are shown by gray-scale plots of Q_{zz}^2; in black regions the liquid crystals are aligned along the z direction and $Q_{zz} = 0$ in white regions. We find from Figure 1 that the distorted region in white is "compressed" and sticks to the particle, which indicates that the imposed flow aligns the liquid crystals along the z direction, allowing a deviation of the orientation from the z direction only in regions very close to the particle. We also notice that the hedgehog defect is pushed towards the particle, or along the flow direction, although its motion is not large enough. As noted in the Introduction, under an electric or magnetic field, a hedgehog transforms itself to a Saturn ring and Stark and Ventzki [16] expected that such a transition might occur under a hydrodynamic flow with a large Ericksen number. In the present simulation, however, we do not observe a transition from a hedgehog to a Saturn ring.

In Figure 2 we show the time evolution of the orientation profile where the flow direction is from the particle to the hedgehog, opposite to that in Figure 1. One can observe strong deformations of the

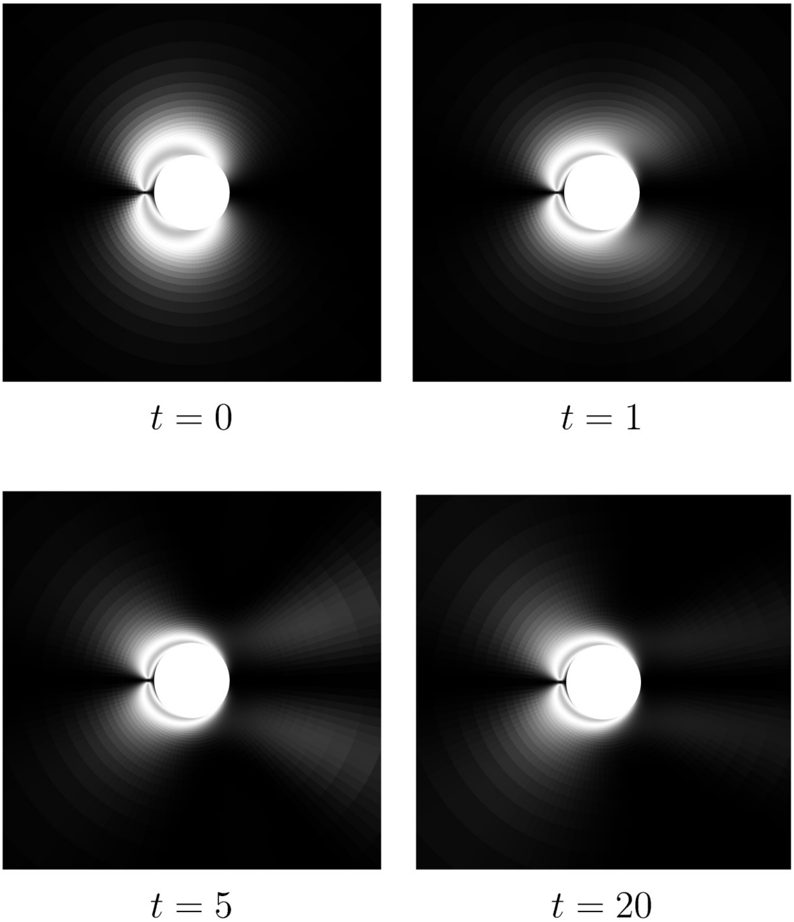

FIGURE 1 Time evolution of the orientation profile from the hedgehog configuration, when a hydrodynamic flow is imposed whose direction is from the hedgehog to the particle (from left to right). The orientation profiles are illustrated by gray-scale plots of Q_{zz}^2. The numbers indicate the time after the application of the flow.

orientation profile together with the motion of the hedgehog defect along the flow direction. Also in this case the hedgehog defect itself looks stable and does not seem to transform itself to a larger ring. We note that the direction of the defect motion is not in agreement with that in a previous study by Stark and Ventzki [16].

Next we present how a Saturn ring is deformed under a hydrodynamic flow. Shown in Figure 3 is the time evolution of the orientation

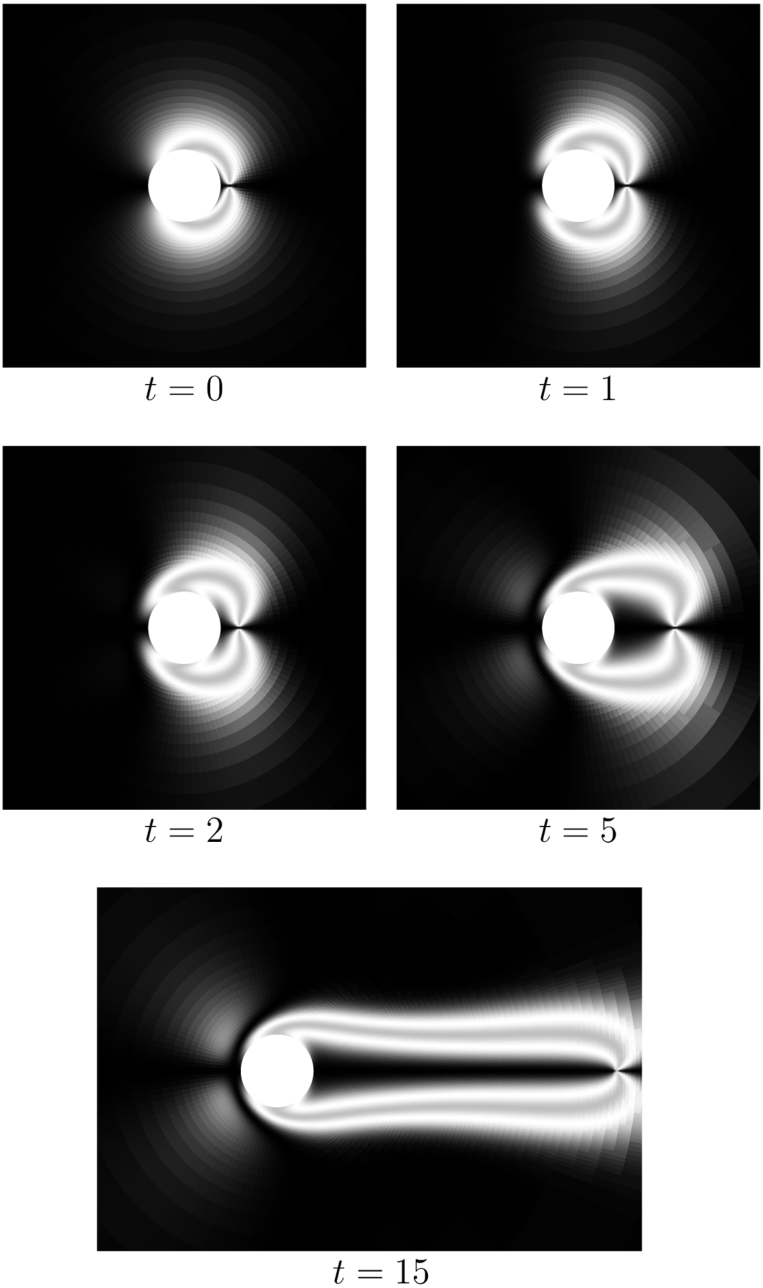

FIGURE 2 Time evolution of the orientation profile from the hedgehog configuration when the flow direction is from the particle to the hedgehog (from left to right).

profile where the flow direction points from left to right. We find that the core of the Saturn ring moves along the flow direction and escapes from the particle. After that the ring defect shrinks and ultimately forms a hyperbolic hedgehog away from the particle. Notice the close resemblance of the orientation profile in Figure 3 at $t = 20$ to that in Figure 2 at $t = 15$.

IV. CONCLUDING REMARK

We investigated numerically the effect of a hydrodynamic flow on the configuration of a nematic liquid crystal around a spherical particle with rigid normal surface anchoring. We employed a continuum description of the orientational order in terms of a second-rank tensor order parameter $Q_{\alpha\beta}$, which enables one to deal with topological defects without introducing any singularities. As a first trial, we made a simplifying assumption of the fixed Stokes flow profile. This assumption greatly reduces the numerical resources necessary for the calculation of the time evolution of the orientational order, because one does not have to solve the equation for the velocity. Then the equation of motion for $Q_{\alpha\beta}$ is easily implemented numerically and we can directly apply an adaptive mesh refinement scheme developed previously to avoid the difficulties arising from the large scale difference between the particle and the defect core. Since we also assumed rotational symmetry of the system, we restricted ourselves to the cases where the flow direction at infinity is along the axis of rotational symmetry.

In the case of the hedgehog configuration as the initial condition, we found that the hedgehog defect moves along the flow direction; when the flow direction is from the defect to the particle, the defect is pushed towards the particle. For opposite flow direction, the defect is pulled away from the particle and considerable elastic deformation of the orientation profile is observed. We did not observe a transition from a hedgehog to a Saturn ring, which was expected in analogy with such a transition under an electric or magnetic field. When a Saturn ring is subjected to a flow, the ring defect moves again along the flow direction, escapes from the particle, and finally shrinks to form a hyperbolic hedgehog.

Our results for a hedgehog configuration as an initial condition contradict those of Stark and Ventzki [16] who found that the motion of a hedgehog defect is against the flow direction. They solved the full Ericksen–Leslie equations for the director $\boldsymbol{n}$ and the fluid velocity to obtain the stationary profiles of $\boldsymbol{n}$; the anisotropy of the viscosity is properly taken into account, but the transient behavior of the

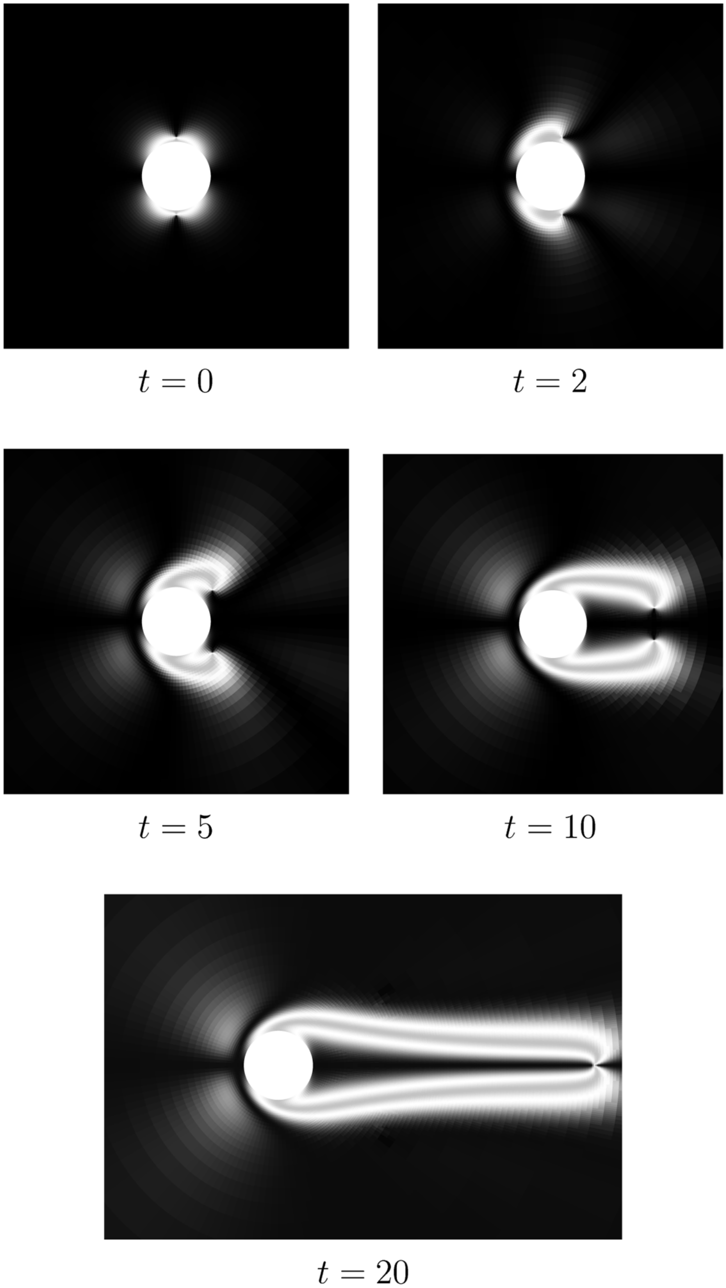

FIGURE 3 Time evolution of the orientation profile from the Saturn ring configuration. The flow direction is from left to right.

orientational order is not argued. On the other hand, our approach makes a simplifying assumption of a Stokes flow as noted above. Therefore the disagreement between the results of Stark and Ventzki and ours might indicate that the motion of topological defects close to a particle under flow may sensitively depend on the anisotropic nature of the viscosity of the liquid crystal.

So far as we know, there have been no experimental attempts to investigate the effect of a hydrodynamic flow, in particular in large Ericksen number cases, on the orientation profile of a nematic liquid crystal around a particle. From Galilei invariance, the flow and director profiles of a flowing nematic around a fixed particle are equivalent to those of a nematic at rest around a particle moving in the opposite direction, and the latter situation is experimentally more accessible. Stark and Ventzki [16] proposed a falling-ball experiment using a gold particle to achieve a large Ericksen number. A centrifuge might also be used to exert a large force to the particle. An optical tweezer may be another candidate for realizing fast motion of a particle in a liquid crystal. As mentioned above, the motion of a topological defect in a nematic liquid crystal around a particle under a hydrodynamic flow is far from being a trivial problem, and experimental studies are therefore highly encouraged.

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