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Cite as: J. Chem. Phys. 140, 054905 (2014); https://doi.org/10.1063/1.4862953 Submitted: 11 November 2013 • Accepted: 10 January 2014 • Published Online: 04 February 2014

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J. Chem. Phys. 140, 054905 (2014); https://doi.org/10.1063/1.4862953

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Effects of flow on topological defects in a nematic liquid crystal near a colloid

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(Received 11 November 2013; accepted 10 January 2014; published online 4 February 2014)

We perform molecular dynamics simulations of a nematic liquid crystal flowing around a colloidal particle. We study the flow-induced modifications of the topological defects in the liquid crystal due to the presence of the colloid. We show that flow distorts Boojum defects into an asymmetrically larger downstream lobe, and that Saturn ring defects are convected downstream along the flow direction, which is in agreement with experimental observations. Additionally, for a Janus colloid with both parallel and perpendicular patches, exhibiting a Boojum defect and a Saturn ring defect, we find that the Boojum defect facing the upstream direction is destroyed and the Saturn ring is convected downstream. © 2014 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4862953]

I. INTRODUCTION

Colloids dispersed in a nematic liquid crystal (LC) host fluid have attracted considerable attention because of their intriguing properties, such as colloidal self-assembly^{1,2} leading to novel photonic band-gap devices,^{3–5} and to the possibility of selecting or sorting particles depending on their size,⁶ or surface properties.^{7,8}

A nematic LC is characterized by a high degree of orientational order along a specific direction, the director \hat{n}_0 . But introducing a colloid can greatly affect the physical properties of its host, namely, it distorts the orientational order of the nematic LC. The distortion is caused by the alignment of LC molecules on the curved surface of the colloid, and can be measured by the local director field $\hat{n}(r)$. Perturbations of the director field lead to long-range, anisotropic forces, which in turn mediate effective interactions among colloids. Due to the distortions in the orientational order of the nematic LC defect topologies arise around the surface of the colloid. To date, a variety of different defect topologies such as Boojum defects or Saturn rings have been observed.^{9,10} To understand the self-assembly of colloids through the effective forces caused by different defect topologies in a nematic LC host one has to study the topologies themselves.

Modern microfluidic devices use flow to manipulate and control fluids and cargoes.¹¹ Whereas the majority of microfluidic applications is based on isotropic liquids, a novel, flexible approach based on anisotropic fluids, that is, LC's, has already been proposed.¹² Therefore, it is timely and important to understand how hydrodynamic flow affects topological defects.

However, the effect of flow on the defect topologies has so far received only moderate scientific attention. Billeter and Pelcovits¹³ performed a falling ball experiment with the aid of molecular dynamics (MD) simulations. They could show that high driving forces acting on the colloidal particle distort the Saturn ring defect topology. Stark and Ventzki¹⁴ showed that a hedgehog defect moves upstream. They also predicted that flow could turn a hedgehog defect into a Saturn ring. Later Fukuda et al.¹⁵ and Yoneya et al.¹⁶ could not observe such a transition and found in contrast that the hedgehog defect moves downstream rather than upstream. Yoneya et al.¹⁶ could also show that a Saturn ring is pushed downstream, escaping from the particle and finally shrinking to a hyperbolic hedgehog defect. Araki and Tanaka¹⁷ showed a detachment of the Saturn ring from the colloid, and reported a strong deformation of the Saturn ring when the flow direction is perpendicular to the global director. With numerical simulations Zhou et al.¹⁸ showed that flow sweeps a hedgehog defect and Saturn ring downstream. Khullar et al.¹⁹ have performed the only experimental study we are aware of. They found that defect structures around rising bubbles and droplets move downstream, and also observed the transition from a Saturn ring into a hedgehog defect. However, Gettelfinger et al.²⁰ recently reported MD simulations showing that the Saturn ring around a solid nanoparticle moves upstream, contradicting Refs. 15-19, while the Saturn ring around a nanodroplet moves downstream. There is, therefore, still some disagreement on the direction of motion of the defect structures around a colloid.

Here, we present nonequilibrium MD simulations of a nematic LC flowing around a spherical colloidal particle. We pay particular attention to the computational challenges of applying a thermostat in a highly nonequilibrium state. If we are to trust the results of computer simulations, we need an efficient way of removing viscous heat from the fluid without introducing artificial dynamical states (an early example of these artifacts is Ref. 21). The Nosé-Hoover thermostat^{22–24} is immediately ruled out because of its global nature. It would remove kinetic energy from regions of low viscous stress

to compensate for the high viscous heating on the upstream side of the colloid. We adopt instead the method of Stoyanov and Groot,^{25,26} which uses a momentum-conserving pairwise force to control the temperature. This choice appears to us as a flexible and robust method for nonequilibrium MD simulations of spatially inhomogeneous systems. We find from our simulations that a Saturn ring around a solid homogeneous nanoparticle moves downstream and is deformed by the hydrodynamic flow.

We also consider Janus colloids. Experimental and theoretical studies of a Janus colloid dispersed in a nematic LC have led to a variety of new defect topologies.^{27,28} Thus, distortions of a flowing nematic LC on the topological defects generated by a Janus particle may offer other surprises. This work represents the first computational study of a Janus particle immersed in a flowing nematic LC host. The Janus particle consists of a patch enforcing planar anchoring, whereas the rest of the surface enforces homeotropic anchoring. In absence of flow the Janus particle generates a Boojum defect (above the planar patch) and a Saturn ring (above the perpendicular patch). We find that hydrodynamic flow can destroy an upstream Boojum defect and convect the Saturn ring downstream.

The remainder of this work is organized as follows. In Sec. II, we describe the model chosen for the LC and for the colloids studied. In Sec. III, we provide details about the MD algorithm and the numerical implementation. In Sec. IV, we explore some static and dynamic observables useful to characterize the physical state of our system. In Sec. V, we describe our results, and finally in Sec. VI, we discuss our results and summarize our conclusions.

II. MODEL

A. Liquid crystal fluid

The interactions among LC molecules, or fluid-fluid (ff) interactions, are described by the Hess-Su²⁹ model potential energy

$$u_{ff}(\boldsymbol{r}_{ij}, \hat{\boldsymbol{u}}_i, \hat{\boldsymbol{u}}_j) = 4\varepsilon_{ff} \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \times \{1 + \Psi(\hat{\boldsymbol{r}}_{ij}, \hat{\boldsymbol{u}}_i, \hat{\boldsymbol{u}}_j)\} \right], \quad (1)$$

where ε_{ff} is our unit of energy throughout this work, $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$ is a distance vector between the centers of mass of molecules *i* and *j*, $\hat{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/r_{ij}$ and $r_{ij} = |\mathbf{r}_{ij}|$ is the magnitude of the distance vector. The orientation of molecule *i* is described by a unit vector $\hat{\mathbf{u}}_i$. Equation (1) is a modified Lennard-Jones potential where the attractive term depends on the orientations of the molecules. In fact, the LC molecules deviate only slightly from a spherical shape, and σ is effectively the diameter. The anisotropy of the model stems from the interaction rather than its elongated shape and is accounted for by the function

$$\Psi(\hat{\boldsymbol{r}}_{ij}, \hat{\boldsymbol{u}}_i, \hat{\boldsymbol{u}}_j) = 5\varepsilon_1 P_2(\hat{\boldsymbol{u}}_i \cdot \hat{\boldsymbol{u}}_j) + 5\varepsilon_2 [P_2(\hat{\boldsymbol{u}}_i \cdot \hat{\boldsymbol{r}}_{ij}) + P_2(\hat{\boldsymbol{u}}_j \cdot \hat{\boldsymbol{r}}_{ij})], \quad (2)$$

where $\varepsilon_1 = 0.04$ and $\varepsilon_2 = -0.08$ are anisotropy parameters and $P_2(x) = (3x^2 - 1)/2$ is the second Legendre polynomial. The anisotropy function Ψ preserves the head-tail symmetry of the molecules, i.e., $\hat{u}_i \leftrightarrow -\hat{u}_i$. The simplicity of the Hess-Su model makes it well suited for computer simulations and it has been successfully used to study and characterize LC phases.^{30–35} It is worth noting that to compare with experiments a single Hess-Su particle should be thought of as a nearly spherical group of elongated liquid crystal molecules.³⁰

The molecules are confined between two planar atomistic substrates in the *z*-direction. The interaction between the fluid and the substrate (fs) is described by the model potential

$$u_{fs}(\boldsymbol{r}_{ij}, \boldsymbol{\hat{u}}_i) = \varepsilon_{fs} \rho_s \sigma^2 \left[\frac{2}{5} \left(\frac{\sigma}{r_{ij}} \right)^{10} - \left(\frac{\sigma}{r_{ij}} \right)^4 g(\boldsymbol{\hat{u}}_i) \right], \quad (3)$$

where the parameter $\varepsilon_{fs} = 5 \varepsilon_{ff}/3$ and $\rho_s \sigma^2 \approx 1.1$ is the areal density of a single layer of substrate molecules. In Eq. (3)

$$g(\hat{\boldsymbol{u}}_i) = (\hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{e}}_x)^2 \tag{4}$$

determines the preferential molecular orientation at the solid surface, the so-called anchoring function, and $\hat{\boldsymbol{e}}_x$ is a vector pointing along the *x*-axis in a space-fixed Cartesian coordinate system. This anchoring function enforces a far-field director $\hat{\boldsymbol{n}}_0$ parallel to the *x*-axis. This is comparable to a typical experimental setup.³⁷

B. Homogeneous colloid

In our simulations, we consider one colloidal particle fixed in space at the center of the simulation box. This corresponds to an experimental setup where optical tweezers are used to fix a colloid in space.^{10,36} We use a slightly modified Lennard-Jones potential to describe the interaction between the fluid and the colloid (fc)

$$u_{fc}(\boldsymbol{r}_i, \boldsymbol{\hat{u}}_i) = 4\varepsilon_{fc} \left[\left(\frac{\sigma}{r_i - r_0} \right)^{12} - \left(\frac{\sigma}{r_i - r_0} \right)^6 g_h(\boldsymbol{\hat{r}}_i, \boldsymbol{\hat{u}}_i) \right],$$
(5)

where \hat{r}_i is the unit vector between the centers of mass of a molecule and the colloid, $r_0 = 3\sigma$ is the hard-core radius of the colloid and ε_{fc} denotes the strength of the interaction. We consider homogeneous colloids with either planar or perpendicular anchoring, which is realized by specifying the form of $g_h(\hat{r}_i, \hat{u}_i)$. We choose

$$g_{\parallel}(\hat{\boldsymbol{r}}_i, \hat{\boldsymbol{u}}_i) = (1 - |\hat{\boldsymbol{u}}_i \cdot \hat{\boldsymbol{r}}_i|)^2, \tag{6}$$

$$g_{\perp}(\hat{\boldsymbol{r}}_i, \hat{\boldsymbol{u}}_i) = (\hat{\boldsymbol{u}}_i \cdot \hat{\boldsymbol{r}}_i)^2, \qquad (7)$$

where Eqs. (6) and (7) correspond to planar and perpendicular anchoring, respectively. We use $\varepsilon_{fc} = 2\varepsilon_{ff}$ for the perpendicular anchoring, but $\varepsilon_{fc} = 4\varepsilon_{ff}$ for the planar anchoring. This is due to the fact that perpendicular anchoring is energetically favored on surfaces and therefore one has to increase the depth of the potential well to favor planar anchoring.

C. Janus colloid

To model Janus colloids^{38,39} one has to consider at the same time two different patches with planar and perpendicular anchoring to the surface.²⁸ This can be achieved by replacing g_h in Eq. (5) with

$$g_J(\hat{\boldsymbol{r}}_i, \hat{\boldsymbol{u}}_i) = \omega_{\parallel} g_{\parallel}(\hat{\boldsymbol{r}}_i, \hat{\boldsymbol{u}}_i) + \alpha \omega_{\perp} g_{\perp}(\hat{\boldsymbol{r}}_i, \hat{\boldsymbol{u}}_i), \qquad (8)$$

where Eqs. (6) and (7) are used and $0 \le \alpha \le 1$ is a dimensionless parameter to weaken the (normally preponderant) perpendicular anchoring. Throughout this work we use $\alpha = 0.5$. In Eq. (8), the anchoring functions are weighted according to

$$\omega_{\parallel} = 1 - \gamma_{\parallel} (1 + \hat{\boldsymbol{r}}_i \cdot \hat{\boldsymbol{e}}_x)^{1/2}, \qquad (9)$$

$$\omega_{\perp} = 1 - \gamma_{\perp} (1 - \hat{\boldsymbol{r}}_i \cdot \hat{\boldsymbol{e}}_x)^2, \qquad (10)$$

where $\gamma_{\,\|} \leq 2^{-1/2}$ and $\gamma_{\,\perp} \leq 0.25$ to guarantee that $\omega_{\,\|}$ and $\omega_{\,\perp}$ be larger than or equal to zero. We choose $\gamma_{\parallel} = 0.7$ and γ_{\perp} = 0.05 to guarantee a rather smooth and numerically stable transition between the two patches. This choice of parameters corresponds to a planar-anchoring patch of about 13% of the total spherical surface. We choose a Janus colloid of the same radius $r_0 = 3.0\sigma$ as the homogeneous colloid. The plane of the equator of the colloid is perpendicular to the versor $\hat{\boldsymbol{e}}_x$ and $\mathbf{r}_i \cdot \hat{\mathbf{e}}_x = +1(-1)$ defines the right (left) hemisphere of the colloid. The position and orientation of the colloid are kept fixed in all simulations. The weighting function $\omega_{\parallel}(\hat{r}_i)$ (Eq. (9)) assumes a maximum on the left hemisphere of the colloid, whereas $\omega_{\perp}(\hat{r}_i)$ (Eq. (10)) has the opposite behavior and reaches its maximum on the right hemisphere of the colloid. Furthermore, changing the exponents in Eqs. (9) and (10) controls the relative size of the two different patches.

III. NUMERICAL DETAILS

A. Simulation protocol

We perform MD simulations of $N = 12\,000$ molecules at a pressure P = 1.8 and temperature T = 0.9 that define an equilibrium thermodynamic state well into the nematic phase. A simulation box with volume $V = l_x l_y l_z \approx (24.0\sigma)^3$ is used to eliminate confinement effects on the defect structures around the colloid ($r_0 = 3.0\sigma$) resulting in a mean number density $\bar{\rho} \approx 0.85$. For the computation of local quantities we discretize our system into cubes with a side length of 0.2σ . Every simulation is performed according to the following protocol: (i) we equilibrate the system composed of LC and colloid in the *NPT* ensemble without flow; (ii) a hydrodynamic flow is applied and a second equilibration run is performed in the *NVT* ensemble to reach the steady state; and (iii) finally, we perform the production run in the *NVT* ensemble, and calculate all physical observables discussed below.

A homogeneous, external body-force F_e is generally sufficient to induce hydrodynamic flow in a MD simulation of a homogeneous system. However, the presence of the colloid in our system breaks translational invariance, so that applying a homogeneous body-force to molecules located in the slipstream of the colloid would be somewhat artificial. Therefore, we restrict the application of the body-force to molecules in a three-dimensional slice of width 2σ in the

x-direction, located upstream of the colloid. This guarantees that molecules are still flowing along the *x*-direction but molecules are not dragged out of the slipstream. One can interpret this as the remaining molecules being pushed by the accelerated molecules.

In the remainder we adopt a Cartesian coordinate system where the confining walls are located at $z = \pm l_z/2$ and periodic boundary conditions are applied in the *x*- and *y*-directions. In all simulations presented here we choose $F_e = F_e \hat{e}_x$; thus, the direction of the flow is parallel to the *x*-axis. In our simulations, we employ a slightly modified version of the velocity-Verlet algorithm to gain more computational efficiency. Therefore, we follow Ref. 40 and implement their algorithm to calculate velocities, rotational velocities, and orientations. Throughout our simulations we use an MD time step $\delta t = 10^{-3}$.

B. Galilean-invariant thermostat

For MD simulations the natural thermodynamic ensemble is the microcanonical ensemble, where number of molecules N, volume V, and energy E are conserved. To perform simulations under constant temperature T one has to implement a thermostat. A common choice is the Nosé-Hoover thermostat.^{22–24} This thermostat has a global nature, because the temperature is regulated through the total kinetic temperature. The thermostat is also non-Galilean invariant, because all calculations are performed in the reference frame where the system's barycenter is at rest. Therefore, this thermostat does not conserve momentum locally. A straightforward implementation of the Nosé-Hoover thermostat is not suitable when external forces acting on the system set a macroscopic fluid flow into motion.

There have been modifications of the Nosé-Hoover thermostat to make it local and thus also conserve local momentum. One simple way of doing this is to separate the system into slices and to apply an isolated Nosé-Hoover thermostat to each slice.^{41,42} Unfortunately, this modification of the Nosé-Hoover thermostat is not satisfactory for our system. For a system containing LC molecules flowing around a colloid the sliced thermostatted system would lead to artifacts such as freezing. This is due to the fact that the colloid is obviously introducing a spatial inhomogeneity that greatly affects the thermostatting of the slices containing parts of it.

The profile-unbiased thermostat⁴³ is a common choice in nonequilibrium MD. This thermostat needs a fine mesh partitioning the system into cells containing only few molecules. We share the skepticism of Ref. 41 about the appropriateness of a definition of temperature based on few molecules per cell. Only few molecules cannot undergo a large number of collisions necessary to establish local equilibrium. However, the profile-unbiased thermostat correctly points to the necessity of a local control of the temperature.

In this work, we employ a thermostat based on a pairwise interaction that was first introduced by Stoyanov and Groot.^{25,26} This thermostat is local and Galilean invariant and therefore conserves momentum locally. The difference between the Stoyanov-Groot and the Nosé-Hoover thermostat is that the former acts on pairs of molecule while the latter on single molecules. Below, we briefly describe our implementation of the Stoyanov-Groot thermostat.

First, we consider the thermostatting pairwise force acting on the molecules i and j

$$\boldsymbol{F}_{ij}^{th} = \lambda \psi(r_{ij}/r_c) \left[1 - \frac{1}{2} (T_i + T_j)/T_0 \right] \\ \times [(\boldsymbol{v}_i - \boldsymbol{v}_j) \cdot \hat{\boldsymbol{r}}_{ij}] \hat{\boldsymbol{r}}_{ij}/\delta t, \qquad (11)$$

where λ is a thermostat coupling parameter, $\psi = 1 - r_{ij}/r_c$ is a smearing function, r_c is a cutoff radius, v_i is the velocity of particle *i*, T_0 is the target temperature, and T_i is the local temperature of molecule *i*. If the local temperature T_i is lower than the target temperature T_0 , F_{ij}^{th} performs work on the fluid and increases its energy, otherwise F_{ij}^{th} dissipates energy. Note that F_{ij}^{th} vanishes if the target temperature T_0 is reached. A desirable feature of the Stoyanov-Groot thermostat is that F_{ij}^{th} is deterministic and does not need the use of random numbers. This is similar to the Nosé-Hoover thermostat. The coupling parameter λ remains constant during the simulation. The local temperature T_i of molecule *i* in Eq. (11) is calculated by

$$k_{\rm B}T_i = \frac{\sum_{j} \zeta(r_{ij}/r_c) \,\mu \,(\boldsymbol{v}_i - \boldsymbol{v}_j)^2}{3 \sum_{j} \zeta(r_{ij}/r_c)},\tag{12}$$

where we choose the smearing function $\zeta = \psi$ (in principle the smearing function and the cutoff radius r_c for the thermostatting force and the local temperature could be different), $\mu = m/2$ is the reduced mass, *m* is the molecular mass, and k_B is the Boltzmann constant. Throughout this work we use $\lambda = 0.3$ and $r_c = 1.2$. The sums in Eq. (12) run over all particles *j* subject to the condition $i \neq j$.

IV. STATIC AND DYNAMIC OBSERVABLES

A. Local nematic director

To compute the local director field $\hat{n}(r)$ we consider the local alignment tensor^{44,45}

$$\boldsymbol{Q}(\boldsymbol{r}) \equiv \frac{1}{2\rho(\boldsymbol{r})} \sum_{i=1}^{N} \left\langle \left[3\hat{\boldsymbol{u}}_{i}(\boldsymbol{r}_{i}) \otimes \hat{\boldsymbol{u}}_{i}(\boldsymbol{r}_{i}) - \boldsymbol{I} \right] \delta(\boldsymbol{r} - \boldsymbol{r}_{i}) \right\rangle,$$
(13)

where " \otimes " is the dyadic product, δ is the Dirac δ -function, I is the unit tensor, and angular brackets indicate the ensemble average. Therefore, $Q(\mathbf{r})$ is a real, symmetric, and traceless second-rank tensor which can be represented by a 3×3 matrix. To calculate the local nematic order parameter one has to solve the eigenvalue equation $Q(\mathbf{r}) \cdot \hat{\mathbf{n}}_n(\mathbf{r}) = \lambda_n(\mathbf{r})\hat{\mathbf{n}}_n(\mathbf{r})$ where λ_n is the *n*th eigenvalue and $\hat{\mathbf{n}}_n(\mathbf{r})$ the associated eigenvector. The three eigenvalues $\lambda_-(\mathbf{r}) < \lambda_0(\mathbf{r}) < \lambda_+(\mathbf{r})$ can be obtained numerically. One can define the local nematic order parameter $S(\mathbf{r})$ as the largest eigenvalue $\lambda_+(\mathbf{r})$ and the associated eigenvector as the local director $\hat{\mathbf{n}}(\mathbf{r})$.

B. Elastic constants

In the hydrodynamic limit a LC can be described by the elastic constants emerging from a continuum description.⁴⁶ To calculate the elastic constants of our system we follow Refs. 47–49. This calculation requires the Fourier transform of the alignment tensor Q(r)

$$\hat{\boldsymbol{Q}}(\mathbf{k}) = \int \boldsymbol{Q}(\boldsymbol{r}) \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) \,\mathrm{d}^{3}\boldsymbol{r}. \tag{14}$$

We define a coordinate system a, b, c such that Q(r) is diagonal and the local director is $\hat{n}(r) = (0, 0, 1)$. For a wave vector $\mathbf{k} = (k_1, 0, k_3)$ in the 1–3 plane the fluctuations are⁵⁰

$$E_{13}(k_1^2, k_3^2) \equiv \frac{9}{4} \frac{S^2 V k_B T}{\langle |\hat{Q}_{13}(\boldsymbol{k})|^2 \rangle} = K_1 k_1^2 + K_3 k_3^2, \quad (15)$$

$$E_{23}(k_2^2, k_3^2) \equiv \frac{9}{4} \frac{S^2 V k_B T}{\langle |\hat{Q}_{23}(\boldsymbol{k})|^2 \rangle} = K_2 k_1^2 + K_3 k_3^2, \quad (16)$$

where S is the nematic order parameter and K_1 , K_2 , and K_3 , are the splay, twist, and bend constants, respectively, in the Frank free energy

$$\mathcal{F} = \frac{1}{2} [K_1 (\nabla \cdot \hat{\mathbf{n}})^2 + K_2 (\hat{\mathbf{n}} \cdot \nabla \times \hat{\mathbf{n}})^2 + K_3 (\hat{\mathbf{n}} \times \nabla \times \hat{\mathbf{n}})^2].$$
(17)

The approximation of linearity in k_1^2 and k_3^2 of Eqs. (15) and (16) is only valid in the limit of small *k* because the elastic constants are only defined for long wavelength director fluctuations. The values at the origin $E_{13}(0, 0)$ and $E_{23}(0, 0)$ should be manually set to zero rather than obtaining them from the simulation, because $E_{13}(0, 0)$ and $E_{23}(0, 0)$ vanish only as $V \rightarrow \infty$.^{47–49}

To obtain k_1^2 and k_3^2 bulk simulations are performed at constant V and T with neither a colloid nor flow for different values of N and V, while keeping the number density $\bar{\rho} \approx 0.85$ fixed. In Figs. 1(a) and 1(b), we show the dependence of E_{13} and E_{23} on k_1^2 and k_3^2 . As predicted from the theory, a linear fit can be applied for not too large values of the wavevectors. We note that the slopes of the two fits are almost identical. In our calculations we find elastic constants $K_1 \approx K_2 \approx K_3$ $\approx K \approx 1.6 \varepsilon_{\rm ff} / \sigma$. The fact that the observed elastic constants of our system are equal, within statistical accuracy, is due to the rather small asphericity of LC molecules in the Hess-Su model. Usually, the elastic constant K_3 is higher than the elastic constants K_1 and K_2 .⁴⁷ But for molecules of nearly spherical shape the bend configuration is energetically more or less equal to the splay and twist configuration. This is obviously not the case for much more elongated molecules that are truly anisotropic in shape, as is the case for the Gay-Berne model of LCs.47-49

C. Dynamic viscosity

An important quantity that will help us to characterize the dynamic state is the dynamic viscosity. From the Navier-Stokes equation within the weak-flow limit for planar Poiseuille flow of a uniform fluid with a constant $\bar{\rho}$ and



FIG. 1. Dependence of $E_{13}(k_1^2, k_3^2)$ (black circles) and $E_{23}(k_2^2, k_3^2)$ (red squares) on (a) k_1^2 for $k_3^2 = 0$ as well as on (b) k_3^2 for $k_1^2 = 0$.

dynamic viscosity η one can derive^{51–53} the steady-state streaming velocity

$$v_x(z) = -\frac{\bar{\rho}F_e}{2\eta} \left[z^2 - \frac{l_z}{4} \right],\tag{18}$$

where F_e is the external driving force acting on the system and l_z is the distance between the two stationary walls in *z*direction. Thus, we can calculate η by fitting the velocity profile with a second-order even polynomial $v_x(z) = c_2 z^2 + c_0$, hence $\eta = -\bar{\rho} F_e/2c_2$. To generate a streaming velocity profile *NVT* simulations without a colloid for different external driving forces F_e were performed. The simulation box is separated into slices of constant volume $l_x l_y \Delta z$, where l_x and l_y represent the box length in the *x*- and *y*-directions and Δz $= 0.2\sigma$. Figure 2 shows the velocity profiles obtained with the recipe just described. A second-order polynomial provides a reasonably good fit of $v_x(z)$. From the fit we find $\eta \approx 50 \sqrt{\varepsilon_{ff} m}/\sigma^2$).

D. Dimensionless measures of flow

Two key dimensionless quantities that can precisely characterize our systems are the Reynolds number \mathcal{R} , which is widely used in fluid mechanics, and the Ericksen number \mathcal{E} , which is common in the field of LCs. Introduced by Stokes⁵⁴ and established by Reynolds⁵⁵ the Reynolds number is a measure of the ratio of inertial to viscous forces



FIG. 2. Streaming velocity profile for external driving forces $F_e = 0.1$ (circles), $F_e = 0.2$ (squares), $F_e = 0.3$ (diamonds), $F_e = 0.4$ (triangle up), $F_e = 0.5$ (triangle down) and corresponding second-order polynomial fits (dashed lines). For the sake of clarity we show every third data point.

where v_{∞} is the streaming velocity at steady state and *l* is the characteristic length of the system. We choose the distance between the two confining walls $l_z = 24\sigma$ as the typical length scale of our system.

The Ericksen number is a measure of the deformation of the director field under flow. Following Refs. 14 and 56, we define \mathcal{E} as the ratio of viscous forces $(\eta v_{\infty}/l^2)$ and the elastic forces (K/l^3) in the momentum balance of the Navier-Stokes equation

$$\mathcal{E} = \frac{\eta v_{\infty} l}{K},\tag{20}$$

where K represents an average Frank elastic constant.

In Table I, we list \mathcal{R} and \mathcal{E} for the flow regime studied in this work. Streaming velocities v_{∞} are obtained from *NVT* simulations of the confined LC fluid in the presence of the homogeneous colloid for different external driving forces F_e . This leads to Reynolds numbers $0.041 \leq \mathcal{R} \leq 0.241$, indicating that the conditions of all our simulations pertain to the laminar flow regime. The measured Ericksen numbers $75.0 \leq \mathcal{E} \leq 443.5$ emphasize a dominant effect of viscous forces over elastic forces.

One should bear in mind that the magnitude of the dimensionless quantities strongly depends on what one chooses as the typical length scale of the system. In previous studies^{16,20} the radius of the colloid is often used as the typical length scale. This leads to smaller dimensionless quantities than the ones presented here. We use the confinement length scale, more specifically the box length l_z , to measure dimensionless quantities of flow. In our opinion a length scale based on the

TABLE I. Reynolds numbers \mathcal{R} and Ericksen numbers \mathcal{E} for different external driving forces F_e and corresponding streaming velocities v_{∞} used in our simulations.

F _e	v_∞	R	£
0.1	0.10	0.041	75.0
0.2	0.22	0.090	165.0
0.3	0.31	0.126	232.5
0.4	0.44	0.180	330.0
0.5	0.59	0.241	443.5

radius of the colloidal particle would be more suitable for a physical situation where a colloidal particle (liquid droplet) is deformed.¹⁸

V. RESULTS

A. Homogeneous colloid

Figures 3(a)-3(c) show three-dimensional representations of the defect structures around a homogeneous colloid with planar anchoring for different Ericksen numbers \mathcal{E} . We mark only locations with a local nematic order parameter $S(\mathbf{r}) \leq 0.2$, which we arbitrarily choose to represent the defect structures. Figures 3(d) and 3(e) show cross-sectional maps of the local nematic order parameter $S(\mathbf{r})$ and of the local director $\hat{\mathbf{n}}(\mathbf{r})$ for the same conditions as in Figs. 3(a)-3(c). The cross-sections are taken along the *x*-*z*-plane that goes through the center of the defect topologies.

Colloidal suspensions of a homogeneous colloid with planar local anchoring in a nematic LC are known to form Boojum defects.⁹ Figure 3(a) shows that in the system at rest $(\mathcal{E} = 0)$ a Boojum defect topology arises due to the strong planar anchoring of the molecules on the colloidal surface. This is indicated as well by the low values of $S(\mathbf{r})$ on the left (negative *x*-axis) and right (positive *x*-axis) sides of the colloid in Fig. 3(d). In these areas $\hat{\mathbf{n}}(\mathbf{r})$ is oriented planar to the colloidal surface, and therefore perturbs the global director field $\hat{\mathbf{n}}_0$.

For $\mathcal{E} > 0$, the upstream lobe of the Boojum defect shrinks, see Figs. 3(b) and 3(c), because the molecules on the upstream side of the colloid are squeezed more tightly against

the colloid with increasing \mathcal{E} which results in their enhanced ordering; at the same time the lobe of the Boojum defect in slipstream of the colloid grows in size because molecules are locally decompressed in the slipstream, resulting in a disordering effect. Figures 3(e) and 3(f) show in detail the compression of the upstream Boojum lobe and the expansion of the slipstream one.

Figure 4 is as Figure 3 but for the case of perpendicular anchoring. When homogeneous colloids with perpendicular anchoring are dispersed in a nematic LC they are known to form Saturn ring defect structures.¹⁰ When no external driving force is applied ($\mathcal{E} = 0$) a Saturn ring defect topology arises around the colloid, because of the strong perpendicular anchoring applied in our simulations (Fig. 4(a)). The Saturn ring defect topology is also indicated by the low values of $S(\mathbf{r})$ at the north and south pole of the colloid (Fig. 4(d)). In these areas the director field is strongly distorted because the anchoring opposes the far-field director.

Our MD simulations show that for $\mathcal{E} > 0$ the defect structures (Figs. 4(b) and 4(c)) are distorted and convected along with the flow in *x*-direction. This is also indicated by the position of the area of low nematic order in Figs. 4(e) and 4(f). This contradicts the results found by Gettelfinger *et al.*²⁰ but is in agreement with earlier theoretical studies^{16–18} as well as experimental work by Khullar *et al.*¹⁹

As \mathcal{E} increases, the local nematic director $\hat{\boldsymbol{n}}(\boldsymbol{r})$ at the north and south pole of the colloid becomes more and more parallel to the global director $\hat{\boldsymbol{n}}_0$. For $\mathcal{E} > 0$ the Saturn ring defect deforms and moves downstream along the *x*-direction (see Fig. 4(c)). The deformation takes the shape of a wide-open mouth. Therefore, we refer to this



FIG. 3. (a)–(c) A three-dimensional representation of the defect structures ($S(r) \le 0.2$) around a homogeneous colloid (gray sphere). (d)–(f) Cross-section along the x-z plane of the local nematic order parameter S(r), where the color indicates the magnitude of S(r), as well as the local director \hat{n} (r) represented by a black line. Plots are generated for different Ericksen numbers \mathcal{E} for a colloid with planar anchoring and the black arrow indicates the direction of the streaming velocity v_{∞} .



FIG. 4. (a)–(c) A three-dimensional representation of the defect structures ($S(r) \le 0.2$) around a homogeneous colloid (gray sphere). (d)–(f) Cross-section along the x-z plane of the local nematic order parameter S(r), where the color indicates the magnitude of S(r), as well as the local director $\hat{n}(r)$ represented by a black line. Plots are generated for different Ericksen numbers \mathcal{E} for a colloid with perpendicular anchoring and the black arrow indicates the direction of the streaming velocity v_{∞} .

deformation as "stomal defect". Figure 5 shows the reason for this deformation. We calculate the *x*-component of the velocity v_x averaged over a plane perpendicular to the *z*-axis, and study its dependence on *z*. We repeat the calculation for planes perpendicular to the *y*-axis to study the dependence of v_x on *y* as well. On the colloidal surface $v_x(z) > v_x(y)$, that is, the molecule moving between the north (south) pole and the top (bottom) wall move faster than the molecules on the equator of the colloid.

An interaction of the Saturn ring and confining walls was observed in experiments by Khullar *et al.*¹⁹ However, in their case the walls of the experimental cell have a pinning effect on the defect, which, we deduce, drastically reduces the velocity



FIG. 5. Streaming velocity profile for a homogeneous colloid with perpendicular anchoring for a Ericksen number $\mathcal{E} = 443.5$ along the *y*- (squares) and *z*-directions (circles) where blue lines represent the diameter of the colloid. For the sake of clarity we show every second data point.

of the LC fluid between colloid and walls. Thus, the section of the Saturn ring closer to the walls moves slower than the sections at 90° from them.

B. Janus colloid

We also perform MD simulations of a Janus colloid with a planar-anchoring patch on the upstream side and a perpendicular-anchoring patch on the downstream side. The planar patch is smaller than the perpendicular one, although the transition between the different patches is rather smooth.

Figure 6(a) shows that for the system at rest ($\mathcal{E} = 0$) a ring defect topology arises around the equator. This is due to the fact that the patch with perpendicular anchoring covers most of the colloid's surface. However, at the smaller patch with planar anchoring a Boojum defect topology comparable to the defect for the homogeneous colloid with planar anchoring arises. Therefore, this defect topology corresponds to a Boojum ring.^{27,28} This is also indicated by the low values of $S(\mathbf{r})$ at the north and south pole as well as on the upstream side of the colloid [see Fig. 6(d)]. On the north and south pole the global director field is perturbed, which is indicated by the perpendicular orientation of $\hat{n}(r)$ with respect to the colloid surface. On the other hand, $\hat{n}(r)$ is oriented planar with respect to the colloid surface on the upstream side of the colloid and therefore the global director field is perturbed here as well.

For increasing values of \mathcal{E} one can see the ring defect structure moves downstream [see Figs. 6(b) and 6(c)]. This is equivalent to the configuration described above for the



FIG. 6. (a)–(c) A three-dimensional representation of the defect structures ($S(r) \le 0.2$) around a Janus colloid. (d)–(f) Cross-section along the x-z plane of the local nematic order parameter S(r), where the color indicates the magnitude of S(r), as well as the local director $\hat{n}(r)$ represented by a black line. Plots are generated for different Ericksen numbers \mathcal{E} for a colloid favoring planar anchoring (dark gray) on the upstream side and perpendicular anchoring (gray) on the downstream side and the black arrow indicates the direction of the streaming velocity v_{∞} .



FIG. 7. (a)–(c) A three-dimensional representation of the defect structures ($S(r) \le 0.2$) around a Janus colloid. (d)–(f) Cross-section along the x-z plane of the local nematic order parameter S(r), where the color indicates the magnitude of S(r), as well as the local director $\hat{n}(r)$ represented by a black line. Plots are generated for different Ericksen numbers \mathcal{E} for a colloid favoring perpendicular anchoring (gray) on the upstream and planar anchoring (dark gray) on the downstream side and the black arrow indicates the direction of the streaming velocity v_{∞} .

homogeneous colloid with perpendicular anchoring. Figures 6(e) and 6(f) confirm this observation. The region of low nematic order is moving downstream. However, the defect structure on the upstream side of the colloid is completely destroyed for high values of \mathcal{E} [see Fig. 6(c)]. This effect can also be observed in the rapid increase of $S(\mathbf{r})$ [see Figs. 6(e) and 6(f)]. The destruction of the point defect structure is due to the fact that molecules are pushed out of the rather small patch favoring planar anchoring by the strong flow applied to the system.

We note that if the Janus colloid is reversed, and therefore exhibits the planar patch in the downstream direction, the Boojum defect grows in size as \mathcal{E} increases. At the same time the Saturn ring deforms into a stomal defect and slowly merges with the growing Boojum lobe (see Fig. 7).

VI. CONCLUSION

We study the defect topologies arising around homogeneous colloids with either planar or perpendicular anchoring to the colloid's surface dispersed in a confined liquid crystal. This leads to well known defect topologies such as the Boojum defect or the Saturn ring. Here, we focus on the effect of flow on these defect structures. In all our simulations, we employ a flow well situated in the laminar flow regime, meaning low Reynolds numbers. However, we study a range of rather high Ericksen numbers and therefore our system is dominated by viscous forces over elastic forces. Furthermore, we make sure that the distance between confinement and colloid is big enough to guarantee that the confinement is not affecting the topological defect structures.

In our calculations we find that for our model system the elastic constants in the Frank free energy are equal within numerical precision. This is due to the fact that the anisotropy of our LC model stems from interaction rather than the elongted shape of its molecules. This leads to a rather small aspect ratio of LC molecules. Therefore, the bend configuration is energetically roughly equal to the splay and twist configuration for LC molecules of nearly spherical shape.

To guarantee an adequate treatment of the nonequilibrium conditions of our system, we employ a Galileaninvariant thermostat that is based on local pairwise interactions.^{25,26} Therefore, the thermostat conserves momentum locally. Furthermore, it is completely deterministic and thus suitable for MD simulations.

The question of the direction of movement of the defect structures does not seem to be completely settled, because there are still some results²⁰ contradicting experimental work¹⁹ and earlier theoretical studies.^{16–18} Our MD simulations show that in fact flow has a significant impact on defect structures around a colloidal particle. In a Boojum defect topology the upstream lobe is swept away by the flow, while the downstream lobe grows in size as \mathcal{E} grows. A Saturn ring is instead convected downstream and deformed into a stomal defect. Our results are in agreement with the experimental observations¹⁹ that Saturn ring defects move downstream accompanied by a deformation of the defect.

We also study flow-induced modifications of topological defects generated by Janus colloids.²⁸ We find that hydrody-

namic flow can destroy a Boojum lobe when it faces the upstream direction, and that a Saturn ring is deformed into a stomal defect.

ACKNOWLEDGMENTS

We thank M. Melle (Technische Universität Berlin), S. Schlotthauer (Technische Universität Berlin), and A. Sengupta (Max-Planck-Institut für Dynamik und Selbstorganisation Göttingen) for helpful discussions. Financial support by the Deutsche Forschungsgemeinschaft (DFG) within the framework of the International Graduate Research Training Group 1524 is gratefully acknowledged.

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