Dynamics of a disclination point in smectic-C and -C^* liquid-crystal films

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We derive a dynamical equation for the stochastic motion of a vortexlike point disclination in thin smectic-C and -C^* liquid-crystal films. The inertial mass results from flow-induced distortions of the director structure in the core region, while the friction force is due to energy dissipation accompanying director rotations. The elastic force obtained from the curvature energy turns out to be negligible. The resulting dynamics is a Brownian motion, where the diffusion constant is much larger than for a comparable physical particle.

I. INTRODUCTION

The number of experimental and theoretical investigations of smectic-C^* liquid crystals has increased very much in the last few years, because of their very interesting electro-optical properties.[1] Progress in film preparation[2] and in optical detection technique[3] has led to a number of new and exciting experimental results, which are important for possible applications as well as for basic scientific research. Here we will try to explain theoretically the motion of a disclination point in smectic-C and -C^* liquid-crystal films, which was observed experimentally[4,5] and simulated numerically[6] recently. The purpose of this paper is not only to give a theory for this experiment, but also to demonstrate that it is possible, starting from the proper hydrodynamic equations of the liquid-crystal phase, to arrive at an equation of motion for a single-defect structure.

Smectic-C and -C^* liquid crystals are characterized by a constant tilt angle θ between $\hat{\mathbf{p}}$, the normal of the smectic layers, and the director $\hat{\mathbf{n}}$ (i.e., the averaged direction of some molecular axis).[7] The projection of $\hat{\mathbf{n}}$ onto the layer plane is called $\mathbf{c}\equiv S\hat{\mathbf{c}}$, with the modulus (order parameter) $S=\sin\theta$. At the phase transition to the smectic-A phase the tilt angle θ and therefore $\mathbf{c}$ vanishes (soft mode). The tilt direction (the direction of $\hat{\mathbf{c}}$) is constant but arbitrary in the C phase, while in the C^* phase it is constant only within every layer but changes helicoidally from layer to layer. In-plane rotations of $\hat{\mathbf{c}}$ (i.e., translations of the helical structure along its axis in the C^* phase) are then the additional hydrodynamic variables.

In a two-dimensional film consisting of only very few layers (ideally only one) there is no difference of the equilibrium structure between the C and the C^* phase. There is, however, a difference with respect to the possible (curvature) elastic deformations of $\hat{\mathbf{c}}$. In addition to the terms quadratic in splay ($\nabla\cdot\hat{\mathbf{c}}$) and bend[8] ($\hat{\mathbf{p}}\cdot\nabla\times\hat{\mathbf{c}}$), the elastic energy contains a linear-bend term in the (chiral) C^* phase, but not in the (achiral) C phase, because $\hat{\mathbf{p}}\cdot\nabla\times\hat{\mathbf{c}}$ is a pseudoscalar quantity.[9] This linear-bend term can also be interpreted as a surface-energy contribution.[10] The existence of linear bend allows for the possibility of a spontaneous bend phase, similar to the way linear twist in chiral nematic liquid crystals[7] or linear splay in polar nematic liquid crystals[11] can lead to a spontaneous twist (cholesteric) and spontaneous splay phase, respectively.

In the experimental situation we will investigate in the following, however, bend is not spontaneous, but is enforced by boundary conditions. Given a circular film (radius R) and a surface treatment that favors $\hat{\mathbf{c}}$ to be tangential to the boundary, the boundary condition in polar coordinates is

$$\hat{\mathbf{c}}(\rho=R)=\pm\hat{\mathbf{e}}_\phi\ , \tag{1.1}$$

which can also be modeled by a surface energy density $-d(\hat{\mathbf{T}}\cdot\hat{\mathbf{c}})^2$, where $d>0$ and $\hat{\mathbf{T}}$ is the unit vector tangent to the boundary. In the C^* phase the linear-bend elasticity will favor one specific sign in Eq. (1.1), which we will assume to be the plus sign in the following. From this boundary condition it is fairly obvious that the $\hat{\mathbf{c}}$ field must have some defects. In the following we will assume that there is just one defect ($+1$ disclination point) and will not touch the question of defect lattices.[12] Since a defect costs energy, there are two possible cases to be distinguished. (i) The core energy is more important than the surface energy fixing $\hat{\mathbf{c}}$ at the boundary (weak anchoring, d small). Then the system will try to get at least partially rid of the defect by shifting it to the surface[10] and violating Eq. (1.1) to some extent. (ii) The surface energy is more important (strong anchoring, $d\to\infty$) and Eq. (1.1) is strictly satisfied. Then the defect stays at the center in equilibrium. We will only deal with the latter case. In Sec. II we briefly summarize the energetics of that situation by discussing the equilibrium structure of the $\mathbf{c}$ field inside and outside the defect core (Sec. II A) and by deriving the elastic restoring force, which acts on a defect displaced from the center (Sec. II B).

In Sec. III the dynamics is explored in a way similar to our treatment of the dynamics of a screw dislocation line in smectic-A liquid crystals.[13] The hydrodynamic equations are solved approximately for the case of a constant flow (a constant motion of the defect in opposite direc-

tion) (Sec. III A). Deformations of the equilibrium $\mathbf{c}$ field due to the flow give rise to an effective mass of the defect (Sec. III B) and dissipation leads to a friction force (Sec. III C). These forces can then be combined to give an effective equation of motion for the defect itself (Sec. III D), which turns out to behave as a Brownian particle. The derivation of the appropriate diffusion constant will be one of the major results of this paper. In an appendix we briefly discuss slightly more general boundary conditions than Eq. (1.1), where the difference between the splay and bend Frank constant cannot be neglected.

II. ENERGETICS

A. Structure

Let us start with the Ginzburg-Landau free energy for the $\mathbf{c}$ vector,

$$\varepsilon_{\mathrm{GL}}=-\frac{a}{2}c^2+\frac{b}{4}c^4+\tfrac{1}{2}k_1(\nabla\cdot\mathbf{c})^2+\tfrac{1}{2}k_2(\hat{\mathbf{p}}\cdot\nabla\times\mathbf{c})^2 -q_0k_2\hat{\mathbf{p}}\cdot\nabla\times\mathbf{c}\ . \tag{2.1}$$

The coefficient a is always positive, since we are in the C or C^* phase; in the smectic-C phase $q_0=0$, while in the C^* phase $q_0>0$ for our choice of the (plus) sign in Eq. (1.1). For S (or θ) constant, Eq. (2.1) reduces to the gradient free energy for $\hat{\mathbf{c}}$ in Ref. 10. Looking for a circular symmetric solution $S=S(\rho)$, it is easy to verify that the pure bend structure

$$\hat{\mathbf{c}}=(-\sin\phi,\cos\phi) \tag{2.2}$$

is a minimum of Eq. (2.1) and satisfies the boundary condition (1.1). The remaining Euler equation for S reads

$$-aS+bS^3+kS\rho^{-2}-k\Delta S=0\ , \tag{2.3}$$

where we have put $k_1=k_2=k$, which is sufficient for the present purpose. Equation (2.3) is solved most conveniently for the two regions, ρ small and ρ large, separately and putting the solutions together at some intermediate ρ_c (called the core radius). For small ρ, S is given by a Bessel function of order one, which starts linearly from zero, thus avoiding any singularity in $\mathbf{c}$ at the origin. Far away from the origin S is constant with a small ρ^{-2} correction. Thus the core of the defect is a region, where the smectic-C or -C^* order parameter gradually decreases ending up with a smectic-A phase at the center. For the director $\hat{\mathbf{n}}$ this means that in the core the tilt angle (with respect to the layer or film normal $\hat{\mathbf{p}}$) goes to zero and at the disclination point $\hat{\mathbf{n}}$ is normal to the film. With respect to $\hat{\mathbf{n}}$ or $\mathbf{c}$ (but not to $\hat{\mathbf{c}}$) this is a nonsingular defect.[14] From a nematic point of view this is a special case for the "escape in the third dimension"[7] despite of the two-dimensional nature of the film. Since the linear-bend elasticity is a surface term and since $\mathbf{c}$ is fixed at the boundary, q_0 does not enter the solution $S(\rho)$ and the equilibrium structure is the same for the C and the C^* phase.

The core radius ρ_c can be determined in two different ways. Either the inside and outside solutions of $S(\rho)$ are put together near the first maximum of the Bessel function such that S and S' are steady, or ρ_c is used as an unknown parameter, with respect to which the total energy of the system is minimized. Fortunately both procedures give roughly the same result, which reads (neglecting numerical factors of order unity and the small ρ-dependent correction outside the core)

$$\tilde{\rho}_c\equiv\rho_c\left[\frac{a}{k}\right]^{1/2}=1 \tag{2.4}$$

and

$$S(\rho)=\begin{cases} S_0\dfrac{J_1(\tilde{\rho})}{J_1(\tilde{\rho}_c)} & \text{for } \rho<\rho_c \\ S_0\equiv\left[\dfrac{a}{b}\right]^{1/2} & \text{for } \rho>\rho_c . \end{cases} \tag{2.5}$$

S_0 is the order parameter of the unconstrained equilibrium phase and is $\approx 0.1-0.5$ for equilibrium tilt angels of $5°-30°$. If we assume that the curvature energy is not influenced by the formation of layers or by the two-dimensional nature of the film, then the Ginzburg-Landau parameter k can be related to the well-known Frank constants of the nematic phase by $k\sim KS_0^{-2}$, where K is of the order of 10^{-7} erg cm^{-1}. Then ρ_c is small (molecular length divided by S_0 or $\approx 100-1000$ Å) except near the phase transition to the smecitic-A phase. With this solution we find the total Ginzburg-Landau energy,

$$\pi^{-1}E_{\mathrm{GL}}=-\tfrac{1}{2}aS_0^2(R^2-\rho_c^2)+kS_0^2\ln\frac{R}{\rho_c}-2q_0kRS_0 +\tfrac{1}{2}\rho_cS_0^2(ka)^{1/2}\ . \tag{2.6}$$

The contributions in (2.6) are related to the outside order parameter field S, the outside curvature of $\hat{\mathbf{c}}$, the linear bend (at the surface), and the $\mathbf{c}$ field inside the core, respectively. Equation (2.6) can be the lower energy minimum (compared to the homogeneous C^* phase with $\mathbf{c}=S_0\hat{\mathbf{e}}_x$), if q_0 is larger than $S_0R^{-1}\ln(R/\rho_c)$. In that case the bend structure described by Eqs. (2.2), (2.4), and (2.5) would occur spontaneously, even without the boundary condition (1.1). Unfortunately q_0 is not related to any parameter in nematic liquid crystals and its magnitude is not known.[15] In the C phase, of course, the boundary condition is crucial for the existence of the defect structure.

B. Elastic force

By symmetry it is obvious that the stable position of the disclination point is in the center of the circular film. Any position out of the center would enhance the energy of the structure and lead to a force acting on the defect. This (elastic) restoring force will be derived now. For displacements of the disclination point, which are small compared to the film radius, we expect that the core region is not affected by the displacement at all. Of course,

this statement can be true only if the core radius ρ_c is much smaller than the film radius R, which we will assume in the following. Then only the (outside) $\hat{\mathbf{c}}$ field (but not S) is changed by the displacement since S (or θ) is position independent outside the core in our approximation. Writing

$$\hat{\mathbf{c}}=(-\sin\Phi,\cos\Phi)\ , \tag{2.7}$$

$\Phi=\Phi(\rho,\phi)$ is determined by the Euler equation $\Delta\Phi=0$, the boundary condition (1.1), and the requirement that near the core $\hat{\mathbf{c}}$ has to be concentric with respect to the new position of the disclination point. For a displacement x_0 (in a direction which we will take as the x direction) the solution is

$$\Phi=\tan^{-1}\frac{y}{x-x_0}+\tan^{-1}\frac{y}{x-(R^2/x_0)}\ . \tag{2.8}$$

It is then straightforward to calculate the total curvature energy[4] outside the core from (2.1),

$$E^{\rm curv}=\pi k S_0^2\left[\ln\frac{R}{\rho_c}+\ln\frac{R^2}{R^2-x_0^2}\right]\ , \tag{2.9}$$

where the first term is the same as in Eq. (2.6). Since $\hat{\mathbf{c}}$ is unchanged at the boundary, the linear-bend energy is not affected by the displacement x_0 like all other contributions in (2.6) as discussed above. The additional curvature energy in (2.9) due to x_0 is, of course, meaningful for $R\gg x_0$ only. The linear elastic restoring force can be read off from (2.9),

$$F_x=-2\pi k S_0^2\frac{x_0}{R^2}\ , \tag{2.10}$$

and is directed towards the center (the stable position). This is a situation where a curvature energy (related to rotational distortions of the phase) is converted into an elastic energy (related to displacements of the defect) since the defect breaks translational symmetry (in the layer plane), which is not broken in the defect-free phase.

III. DYNAMICS

A. Constant motion

We will now study the dynamics of the disclination point. We use the hydrodynamic equations to determine how the static solutions for $\hat{\mathbf{c}}$ and S, Eqs. (2.2) and (2.5), are changed in a dynamic situation. Subsequently, these changes will give rise to inertial and friction forces on the defect. We restrict ourselves to a motion of the defect with constant speed. This is equivalent to a situation where the fixed defect is subject to an imposed constant velocity field. Since displacements of the defect out of the center have already been discussed in the statics, we will assume here that the defect is always centered.

Although the hydrodynamics of smectic C and C^* are completely different from each other in three dimensions due to their different symmetries and different broken symmetries,[16] in a film they are rather similar. Neglecting the thermal degree of freedom, keeping the smectic layers rigid, and not allowing for an electrical field, there are no chiral terms left[17] which would discriminate between the C and the C^* phase. Furthermore, if we neglect possible cross-dissipation terms and the difference between the two flow alignment parameters (in the same spirit we have neglected the difference between the two curvature elastic constants in the statics) the hydrodynamic equations are isomorphic to those in nematic liquid crystals. Using the modulus S and Φ [cf. Eq. (2.7)] as variables, the equations are explicitly

$$\frac{\partial}{\partial t}\Phi+\mathbf{v}\cdot\nabla\Phi+\mathbf{p}\cdot\boldsymbol{\omega}-\frac{\lambda}{2}[\sin(2\Phi)(\nabla_x v_x-\nabla_y v_y)+\cos(2\Phi)(\nabla_x v_y+\nabla_y v_x)]=-\frac{\zeta_1}{S^2}\frac{\delta\varepsilon_{\rm GL}}{\delta\Phi}\ , \tag{3.1}$$

$$\frac{\partial}{\partial t}S+\mathbf{v}\cdot\nabla S=\zeta_2\frac{\delta\varepsilon_{\rm GL}}{\delta S}\ , \tag{3.2}$$

$$\rho_m\left[\frac{\partial}{\partial t}\mathbf{v}+\mathbf{v}\cdot\nabla\mathbf{v}\right]+\nabla p+\tfrac{1}{2}\nabla\cdot\overleftrightarrow{\Lambda}\frac{\delta\varepsilon_{\rm GL}}{\delta\Phi}=\nabla\cdot\overleftrightarrow{\nu}:\nabla\mathbf{v}\ , \tag{3.3}$$

where ρ_m is the mass density, p is the pressure, and incompressibility $\nabla\cdot\mathbf{v}=0$ is assumed. The flow alignment tensor reads

$$\overleftrightarrow{\Lambda}=\begin{pmatrix}\lambda\sin(2\Phi) & 1-\lambda\cos(2\Phi)\\ -1-\lambda\cos(2\Phi) & -\lambda\sin(2\Phi)\end{pmatrix}\ . \tag{3.4}$$

Unlike most other cases, where the relaxation of the modulus and the dissipation of the order parameter structure are completely different processes, here in both cases rotations of $\hat{\mathbf{n}}$ are involved and one can expect $\zeta_1\approx\zeta_2\approx\zeta$, the (inverse) nematic rotational viscosity (sometimes called γ_1^{-1}), which is of the order of 10 cm^3/erg sec.

We cannot solve Eqs. (3.1)–(3.3) in full generality. First, we are only looking for stationary solutions neglecting transients. Second, we assume that the velocity field is just the "external" constant velocity $\mathbf{v}=-c_0\hat{\mathbf{e}}_x$ present in the comoving frame, if $+c_0$ is the speed of the defect in fixed frame. That means we neglect back flow effects, i.e., deviations from the external velocity field due to the $\hat{\mathbf{c}}$ texture in the film. This will be justified *a posteriori*. Under these assumptions there is no shear, rotational, or elongational flow acting on Φ, and only transport changes the equilibrium solutions (2.2) and (2.5) and the governing equations are

$$\alpha\nabla_x\Phi=-\Delta\Phi\ , \tag{3.5}$$

$$\alpha\nabla_x S=-k^{-1}\frac{\delta\varepsilon_{\rm GL}}{\delta S}\ , \tag{3.6}$$

with $\alpha=c_0/\zeta k$. Although Eq. (3.5) is linear, it is impossible to give the solution in a simple form, since Φ not only has to fulfill the boundary condition (1.1), but also has to conserve the Burgers "vector" (or the topological charge) of the defect $\oint\nabla\Phi\cdot d\mathbf{s}=2\pi$, since the topology is not changed by flow. It is easy to give a perturbational solution of (3.5) as a power series in α. This is, however, a singular expansion leading to an asymptotic series at

best. Fortunately, we will not need the complete explicit solution in the following.

We will now show that the neglection of back flow is a self-consistent assumption. Inserting for $\delta\varepsilon_{GL}/\delta\Phi$ in Eq. (3.3), the left-hand side of (3.5) with $\Phi=\phi$, the static solution, it is straightforward to verify that the solution is

$$\mathbf{v}=-c_0\hat{\mathbf{e}}_x \tag{3.7}$$

and

$$p=p_0+(\lambda+1)\frac{S^2c_0}{\zeta}\frac{\cos\phi}{\rho} . \tag{3.8}$$

Thus only the pressure is changed in first order. The next order, where v also would be changed, will never be used here.

B. Effective mass

We are now in the position to derive the effective mass of the dislocation point defect. The simplest approach would be to assign the mass located in the core region as the mass of the defect resulting in $m=\rho_m\pi\rho_c^2$. However, this physical picture is wrong. When the defect moves there is no mass transport involved, since the core is defined as a region, where the tilt angle is different from its equilibrium value. Thus displacing the core means physically just a rotation of $\hat{\mathbf{n}}$ at some regions[18] and the inertia associated with this is not related to the mass density but to the moment of inertia. During such a rotation the tilt angle changes roughly from S_0 to zero in the time ρ_c/c_0. For rodlike molecules the moment of inertia is $(\frac{1}{12})L^2m_{\text{mol}}$, with m_{mol} the molecular mass and L the length of the molecules. The kinetic energy of the rotation of the molecules in the core is then approximately

$$E_{\text{rot}}=\frac{\pi}{24}\rho_m S_0^2L^2c_0^2 , \tag{3.9}$$

giving rise to an inertial force, which is by a factor of $10^{-1}S_0^4$ smaller than the inertial force due to a solid translation of the core (for $\rho_c\approx L/S_0$).

There is, in addition, inertia associated with the deformations of the c structure due to flow. Since in the presence of flow S and Φ are different from their static equilibrium values, the energy of the state is higher. The additional energy is due to flow and its part quadratic in v can be interpreted as a kinetic energy. By symmetry there is no part of the energy linear in v.

Outside the core the modulus S_0 is unchanged, since $S=$const is still a solution of (3.6). The Φ-dependent part of the total energy can then be written

$$2E_\Phi/k=\int S^2(\nabla\Phi)^2dV=S_0^2\oint\Phi\,\nabla\Phi\cdot d\mathbf{f} -S_0^2\int\Phi\,\Delta\Phi\,dV . \tag{3.10}$$

To the second part of the integral, the area outside the core contributes nothing, since by Eq. (3.5) $\Delta\Phi$ can be transformed into $\nabla_x\Phi$ leading to an integral containing only Φ^2 at the boundary, which is, however, not velocity dependent due to Eq. (1.1). The surface integral in (3.10) has to be taken along the boundary $\rho=R$ and around a radial cut, where Φ makes a 2π jump. This jump is required by the topology of the defect and is independent of flow. There is no surface at the core radius, since all functions are smooth there. Using infinite perturbation series for $(\partial\Phi/\partial\rho)_{\rho=R}$ and $(\partial\Phi/\partial\phi)_{\phi=2\pi}$, we find again that (at least in quadratic order in the velocity) the outside region does not contribute to the velocity dependent part of E_Φ.

For the core region, where $\alpha\rho$ is always small, one can use a simple perturbation solution of (3.5) and (3.6) to calculate the velocity-dependent part of the core energy, for which we find

$$E_c=\frac{\pi}{8}kS_0^2\alpha^2\rho_c^2\left[\left[\ln\frac{\rho_c}{R}\right]^2+c_1\ln\frac{\rho_c}{R}+c_2\right] , \tag{3.11}$$

where c_1 and c_2 are numerical factors of order one ($c_1\le c_2$). For $R\gg\rho_c$ the latter terms are negligible. The radius R enters (3.11) because of the boundary condition (1.1).

From Eq. (3.11) an effective mass $m_{\text{eff}}=d^2E_c/dc_0^2$ can be derived,

$$m_{\text{eff}}=\pi\rho_c^2\frac{S_0^2}{4\zeta^2k}\left[\ln\frac{\rho_c}{R}\right]^2 , \tag{3.12}$$

which is much larger than both the inertial mass due to rotations of the molecules and the physical mass of the core region. The effective mass is nonlocalized and stored in the elastic distortions of the c structure due to flow.

C. Friction force

We will now derive the friction force, which acts on the disclination point defect in a constant flow field. We restrict ourselves to that part of the force which is linear in the velocity. We obtain this force from the energy dissipation in the system, which will be discussed first. The rate of dissipated energy can be derived from the thermodynamic Gibbs relation

$$T\,d\sigma=\frac{\partial\varepsilon}{\partial S}dS-\frac{\partial\varepsilon}{\partial\Phi}d\Phi , \tag{3.13}$$

where σ is the entropy density. In Eq. (3.13) we have already omitted the irrelevant degrees of freedom, which we have either neglected generally (like the thermal degree of freedom) or which do not contribute to the entropy production (like the velocity). In our first-order treatment of the dynamics, the velocity field remains constant and undisturbed by the presence of the defect and thus does not lead to any dissipative effect. This absence of viscous friction is a result of the special nature of the defect. Since its core is penetrable by flow (it is a nematic state like the outside region), the flow is undistorted (in first order), and since the motion of the core is not a translation of physical particles (but a rotation), there is no friction force at the core boundary (as it would be for the motion of a solid body). There are, however, dissipative effects due to the rotation of the molecules, which are expressed by the right-hand side of Eqs. (3.1) and (3.2).

The rate of energy dissipation $\dot{\varepsilon}^{\text{diss}} = -T\dot{\sigma}$ then follows from (3.13) and (3.1) and (3.2),

$$\dot{\varepsilon}^{\text{diss}} = \zeta \left[\left[\frac{\delta\epsilon}{\delta S} \right]^2 + k^2 S^2 (\Delta\Phi)^2 \right] . \tag{3.14}$$

The desired lowest-order result is obtained by substituting the lhs of Eqs. (3.5) and (3.6) for $\Delta\Phi$ and $\delta\epsilon/\delta S$ and using then the equilibrium values for $\nabla_x \Phi$ and $\nabla_x S$. The total rate of energy dissipation follows from a straightforward integration over the whole area and is found to be

$$\dot{E}^{\text{diss}} = \pi\zeta^{-1} c_0^2 S_0^2 \left[\ln \frac{R}{\rho_c} + c_3 \right] , \tag{3.15}$$

where c_3 is a numerical factor of order unity.

This energy dissipation rate is due to a motion of the defect with velocity $\mathbf{v} = +c_0 \hat{\mathbf{e}}_x$ and the effective friction force, which tends to oppose the constant motion, is $\mathbf{F} = -\nabla_{\mathbf{v}} \dot{E}^{\text{diss}}$. This effective friction force is a nonlocal force due to the dissipation which accompanies flow induced deformations of the S and Φ fields. In the approximation used, $\mathbf{F} \sim -\mathbf{v}$ and the proportionality factor, the (inverse) mobility μ, can be read off from Eq. (3.15),

$$\mu = 2\pi S_0^2 \xi^{-1} \ln \frac{R}{\rho_c} . \tag{3.16}$$

As expected from the above discussion, μ is proportional to the rotational viscosity and independent of (ordinary) viscosity.

D. Brownian motion

We will now reap the fruits of the efforts of Secs. III A–III C and put together an equation of motion for the disclination point defect. A moving macroscopic object can be described by the balance of forces including the inertial force. For a displacement $x_0(t)$ we can write

$$m\ddot{x}_0 + \mu\dot{x}_0 + f x_0 = m\xi(t) , \tag{3.17}$$

describing the inertial, friction, elastic, and stochastic force, respectively. The stochastic force $\xi(t)$ describes the influence of all the microscopic degrees of freedom, which we do not consider explicitly, on the macroscopic variable x_0. This interaction is included in a stochastic manner only and $\xi(t)$ is assumed to be a Gaussian, white noise, stochastic process,[19] i.e.,

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = \Gamma\delta(t-t') . \tag{3.18}$$

The fluctuation strength Γ is related to the dissipation of the system because we deal with a situation near equilibrium. Splitting the dynamics into a deterministic part [containing only $x_0(t)$] and a stochastic part representing all other degrees of freedom requires a separation of times scales relevant for the two groups of variables. In the present case this requirement means that the hydrodynamic degrees of freedom (flow, director rotations, temperature), which are on a macroscopic time scale just like $x_0(t)$, are not excited except to that extent they are related to the dynamics of $x_0(t)$. Of course, flow and director rotations associated with the motion of the defect are assumed to be taken into account already in Eq. (3.17). Then $x_0(t)$ is indeed the only macroscopic dynamic variable of the system.

With this proviso it is possible to identify the forces in Eq. (3.17) with the appropriate forces derived in Secs. III A–III C: the mass m is the effective mass m_{eff} given in Eq. (3.12), the friction coefficient μ is the inverse mobility of Eq. (3.16), and the elastic constant f is defined in Eq. (2.10) as $2\pi k S_0^2 R^{-2}$. However, these forces were not derived for a general motion of the defect, but for rather restricted situations. First, $x_0 \ll R$ was assumed (for the derivation of the elastic force and implicitly by neglecting flow reflected from the boundary) and clearly this restriction applies to Eq. (3.17) too. Second, the friction and inertial force were only derived for a constant motion of the defect, whereas Eq. (3.17) will be applied to more general motions. Although there seems to be no special problems related to this approximate treatment, it surely restricts a comparison of the solution of Eq. (3.17) with experiment to be qualitative in nature.

The dynamics of the defect contains two natural frequencies $\omega_0 = f/m$ and $\gamma = \mu/m$ connected with oscillation and relaxation, respectively. They are, however, of completely different order of magnitude and

$$\frac{\omega_0}{\gamma} = \frac{\rho_c}{R} \ll 1 , \tag{3.19}$$

rendering the system overdamped. Equation (3.17) can then be simplified into

$$\dot{v}_0 + \gamma v_0 = \xi(t) , \tag{3.20}$$

describing a "Rayleigh particle."[19] The standard solution for this simple stochastic process then reveals that for times larger than the relaxation time, $t \gg \gamma^{-1}$, the velocity correlation function is constant and independent of any initial disturbance

$$\langle v_0(t)^2 \rangle = \frac{k_B T}{md} , \tag{3.21}$$

while the position correlation function is of the Brownian-motion type,

$$\langle x_0(t)^2 \rangle = 2Dt = 2\frac{k_B T}{\mu d} t . \tag{3.22}$$

Here we have made use of the dissipation-fluctuation theorem, $\Gamma = 2\gamma k_B T/md$, where k_B is the Boltzmann constant and d is the thickness of the film.[20] Inserting realistic values ($R = 1$ cm, $\rho_c = 10^2$–10^3 Å), the relaxation time

$$\gamma^{-1} = (\rho_c^2/8\xi k) \ln(R/\rho_c) ,$$

which is roughly the diffusion time of director rotations on a length scale of ρ_c, is indeed very small ($< \mu$sec) and the solutions (3.21) and (3.22) are the relevant ones for macroscopic experiments. Thus the variance of x_0 is only slowly increasing with time, since $D \approx 10^{-6}$ cm^2/sec, and the standard deviation of v_0 is of the order of 1 cm/sec. Comparing with a physical particle of the same mass (and density 1 g/cm^3), subject to a Stokes fric-

tion force, the diffusion constant D of the point defect is 3 orders of magnitude larger. For thick films, where $d=nL$, the mean-squared displacement and the mean-squared velocity decrease $\sim 1/n$ with the number of layers. Preliminary studies show that the above results describe the experiments[5] qualitatively correct, although a quantitative analysis has to be done in the future. The simulation of vortex dynamics in the XY model[6] leads to a dynamics rather similar to Eqs. (3.21) and (3.22), although a detailed comparison is impossible, since mass, interaction, and friction force are of different physical origin in the XY model.

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APPENDIX

In this appendix we briefly comment on the case where the boundary condition is more general than Eq. (1.1), i.e., the $\hat{\mathbf{c}}$ vector makes an angle $\psi_0=$ const other than zero (or $\pi/2$) with the circular boundary. In that case it is necessary to distinguish between the two Frank parameters k_1 and k_2, which we parametrize[10] by $k_1+k_2\equiv 2k$ and $k_1-k_2\equiv 2\beta$. The Ginzburg-Landau Eq. (2.1) then gives rise to two Euler-Lagrange conditions concerning minimization with respect to S and Φ [cf. Eq. (2.7)], respectively. For $\Phi=n\phi+\psi_0$, which describes a disclination of strength n and which fulfills the boundary conditions mentioned above, and for $S=S(\rho)$, the latter condition reads

$$\beta\sin\{2[(n-1)\phi+\psi_0]\}\left[S'^2-\frac{2n}{\rho}SS'+\frac{n(2-n)}{\rho^2}S^2\right]=0\ . \quad \text{(A1)}$$

This condition is satisfied identically (i) for $n=1$, $\psi_0=0$, the case dealt with in the main part of this paper (and where $\beta=0$ does not change anything qualitatively); (ii) for $n=0$, $S=S_0$, the unconstrained smectic-C or-C^* phase, and (iii) for $n=2$, $S=S_0$, the disclination point of strength 2. However, the latter does not fulfill the Euler-Lagrange condition with respect to S,

$$-aS+bS^3+k\left[\frac{n^2}{\rho^2}S-\frac{1}{\rho}S'-S''\right]+\beta\cos\{2[(n-1)\phi+\psi_0]\}\left[\frac{n^2}{\rho^2}S-\frac{(2n-1)}{\rho}S'-S''\right]=0\ , \quad \text{(A2)}$$

and S cannot be constant in this case.

Let us come back to the case $n=1$ and $\psi_0\neq 0$, which we are interested in here. Since the above ansatz does not lead to a solution in that case, a more general form, $\Phi=\phi+\psi(\rho)$, has to be employed. Skipping the lengthy calculations, we state that for large ρ

$$\psi(\rho)=\psi_0+\frac{\beta\sin(2\psi_0)}{2[k-\beta\cos(2\psi_0)]}[\ln(\rho/R)]^2\ , \quad \text{(A3)}$$

which reduces for ψ_0 and $\varepsilon\equiv R-\rho$, both being small, to

$$\psi(\rho)=\psi_0\left[1+\frac{k_1-k_2}{2k_2}\frac{\varepsilon^2}{R^2}\right]\ , \quad \text{(A4)}$$

while inside the core $\psi(\rho)=0$. The length scale, over which ψ changes from ψ_0 to 0,[21] is roughly given by R. The modulus S is qualitatively unaffected by $\psi_0\neq 0$ and is constant for large ρ (with a correction $\sim\rho^{-2}$) and starts linearly $\sim\rho$ for small ρ.

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