Disclination dynamics in nematic liquid crystals

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This paper presents a simple particle plus field model for the dynamics of disclination lines in a nematic liquid crystal. The model has no logarithmic divergences with system size and, therefore, no need to introduce a cutoff. The resulting equation of motion relates the velocity of the disclination to the local phase gradient at the core of the disclination. The equation is used to obtain a solution, with a scaling behavior at small time for the annihilation of a pair of opposite strength disclinations. In addition, this paper develops a criterion for the flow speed required to free a disclination from the boundary constraints of the container. [S0163-1829(96)01633-5]

The mathematical characterization of topological defects and in particular their dynamics has received much recent attention. There are several reasons why nematic liquid crystals are an ideal material for the study of such defects. The first reason is the relative ease with which such defects in liquid crystals can be studied in the laboratory. The second reason is that the behavior of the nematic outside the defect can be well described by a continuum theory of the unit vector field, or director. (This theory was due originally to Oseen[1] and Zocher[2] and later refined by Frank,[3] Ericksen,[4] and Leslie.[5] For a more complete description see also Refs. 6 and 7.) These qualities make liquid crystals convenient for theoretical study. Another reason for some of the recent interest in liquid crystals is that the dynamical equations governing the evolution of the director field find an analog in the nonrelativistic nonlinear σ model, which determines the evolution of global defects produced in cosmology.[8,18]

Recent work, both experimental[9] and theoretical,[10–13] has examined the dynamics and structure of line defects, called disclinations, in nematic liquid crystals. The earliest works on disclination dynamics[14,15] concentrated on calculating a frictional coefficient η, which is related to a drag force $\eta\gamma_1\dot{\mathbf{q}}$, where γ_1 is a viscosity coefficient and $\dot{\mathbf{q}}$ is the disclination velocity. These efforts suffered from a diverging frictional coefficient caused by the failure of the static field equations to accurately describe the field of a moving disclination at large distances from the defect core. (This is also the problem in Ref. 11.) Ryskin and Kremenetsky[10] rectified this problem and obtained a nondivergent η. However, they did not obtain a complete description of the dynamics of the disclination in the form of an equation of motion. Such an equation should include a driving force as well as the drag force. The purpose of this work is to obtain an equation of motion for a line defect moving in a nematic medium.

In the absence of fluid flow, the equation describing the relaxation of the liquid-crystal three-component director field $\mathbf{n}$, in the nematic phase, is[7]

$$\partial_t n_i = -\frac{1}{\gamma_1} h_i, \tag{1}$$

where γ_1 is the twist viscosity. The vector $\mathbf{h}$ is a variational derivative of the elastic free energy and involves a Lagrange multiplier λ, to take into account the auxiliary condition $\mathbf{n}^2 = 1$;

$$\mathbf{h} = \frac{\delta}{\delta \mathbf{n}} \int \{F - \tfrac{1}{2}\lambda(\mathbf{r})\mathbf{n}^2\} d\mathbf{r}, \tag{2}$$

where the deformation energy density $F = \{K_1(\nabla\cdot\mathbf{n})^2 + K_2[\mathbf{n}\cdot(\nabla\times\mathbf{n})]^2 + K_3[\mathbf{n}\times(\nabla\times\mathbf{n})]^2\}/2$.

There is one case in which the field equations simplify greatly. This occurs in the one-elastic-constant-K approximation and where the director lies in a plane $[\mathbf{n} = (\cos\phi, \sin\phi, 0)]$. Comparison of numerical work on coarsening dynamics of the XY model[19] and phase ordering for the entire nematic order parameter[20] shows that this is not an unreasonable restriction, at least in two dimensions. The field equations can now be derived from the following energy functional:[6,16]

$$\mathcal{F} = \int_V \frac{K}{2} (\nabla\phi)^2 d\mathbf{r} \tag{3}$$

and some assumption about the dissipation. Applying the standard approach, as utilized in Eq. (1), leads to the equation

$$\partial_t \phi = -\frac{1}{\gamma_1} \frac{\delta \mathcal{F}}{\delta \phi}. \tag{4}$$

In order to obtain an equation of motion for the disclinations, we proceed as follows. First, we look at the solutions to Eq. (4) which satisfy the topological constraint imposed by a disclination. Then we use the resulting solution, which is only valid outside the core region, as a starting point to take into account the fact that the boundary, as set by the position of the core, is moving.

Consideration of the variation of $\mathcal{F}$ inside the volume V, bounded by the walls of the container and punctured by the core region of any disclination lines present, gives

$$\delta\mathcal{F} = -\int_V \delta\phi \nabla^2 \phi \, d\mathbf{r}. \tag{5}$$

Combined with Eq. (4), this $\delta\mathcal{F}$ leads to a diffusion-type equation

$$\partial_t \phi = D\nabla^2 \phi \tag{6}$$

inside the volume V with a diffusion constant $D=K/\gamma_1$. In the reference frame of a disclination defect placed at $\mathbf{q}(t)$, this becomes

$$D\nabla^2 \phi = \partial_t \phi - \dot{\mathbf{q}} \cdot \nabla \phi, \tag{7}$$

where $\dot{\mathbf{q}}$ is $\partial_t \mathbf{q}$ in the original reference frame. The diffusion equation being linear, we can treat the disclination separately and first solve for the field ϕ_q due to the disclination which satisfies

$$D\nabla^2 \phi_q = -\dot{\mathbf{q}} \cdot \nabla \phi_q, \tag{8}$$

with the boundary conditions

$$\phi_q \rightarrow s\alpha + \text{const} \quad \text{as} \quad (\mathbf{x}-\mathbf{q}) \rightarrow 0. \tag{9}$$

Then $\phi = \phi_q + \phi_{\text{ex}}$ is a solution of Eq. (7) satisfying the topological constraint at $\mathbf{q}$, where the ''external field'' ϕ_{ex} is any solution of the diffusion equation which is analytic over the core region of the disclination at $\mathbf{x}=\mathbf{q}$. The solution to Eqs. (8) and (9) with a disclination of strength s centered at the origin of the moving frame is

$$\phi_q(\mathbf{r}) = \int_0^{\alpha} \left(\nabla g + \frac{1}{D} \dot{\mathbf{q}} g \right) \cdot \hat{\mathbf{r}}' \, d\alpha',$$

$$g(\mathbf{r}) = -s \exp\left(-\frac{1}{2D} \dot{\mathbf{q}} \cdot \mathbf{r} \right) K_0\left(\frac{1}{2D} |\dot{\mathbf{q}}| r \right), \tag{10}$$

where $\mathbf{r}$ is given in polar coordinates (r,α), K_0 (as well as K_1 and I_1 below) is the modified Bessel function, and an arbitrary additive constant has been set to zero. (This is a generalization of the solution given in Refs. 17 and 10 to a disclination moving in any direction.)

The key difference between this and most previous works is that solutions to the diffusion equation, rather than Laplace's equation, are used (i.e., unlike in Ref. 11, ϕ_q does not satisfy the static equation). This avoids numerous logarithmic divergences with the system size. The reason for this is that ϕ_q in Eq. (10) has a *finite* interaction length [taking $r \rightarrow \infty$ with fixed $\dot{q}$, in Eq. (10) gives $\phi \rightarrow 0$]. As we will see below, this interaction length, which depends on $\dot{q}$, can also be used to determine when a disclination will be free of the boundaries of the container in which the liquid crystal sits. So far we have no equation of motion for $\mathbf{q}$. This is due to the neglect of the surface terms in the variation $\delta\mathcal{F}$ given in Eq. (5). The above equations can be extended in a natural way in order to obtain an equation of motion for a disclination. This is done by considering the free energy cost involved in displacing the disclination with respect to the background fields. Note that all volume integrals should be done only over a punctured domain which excludes small regions around the defect cores, and Eq. (4) is replaced by

$$\int_V \delta\phi \partial_t \phi d\mathbf{r} = -\frac{1}{\gamma_1} \delta\mathcal{F}. \tag{11}$$

The key here is that now $\delta\mathcal{F}$ will include terms involving the shift in the position of the finite-sized core region.

Let us now write the energy (3) in terms of the two fields ϕ_q and ϕ_{ex}:

$$\mathcal{F} = \frac{K}{2} \int_V [(\nabla \phi_q)^2 + (\nabla \phi_{\text{ex}})^2 + 2\nabla \phi_q \cdot \nabla \phi_{\text{ex}}] d\mathbf{r}. \tag{12}$$

Consider a virtual displacement, $\delta\mathbf{q}$, of the disclination. In order to maintain correct boundary conditions, we must also displace the field ϕ_q by $\delta\mathbf{q}$. This is equivalent to a functional change in ϕ_q of

$$\delta\phi_q = -\delta\mathbf{q} \cdot \nabla \phi_q. \tag{13}$$

Now consider the individual terms in Eq. (12). There is no change in the integral of the $(\nabla \phi_q)^2$ term as ϕ_q has been displaced, along with the disclination core. The shift in the core position causes a surface term to arise involving the other integrands. Finally, there is a volume integral from the cross terms since ϕ_q has been shifted while ϕ_{ex} has not. The full variation of $\mathcal{F}$ is now

$$\begin{aligned} \delta\mathcal{F} &= K \int_V \nabla \phi_{\text{ex}} \cdot \nabla \delta\phi_q d\mathbf{r} + \frac{K}{2} \int_{\partial V} \boldsymbol{\sigma} \cdot \delta\mathbf{q} [(\nabla \phi_{\text{ex}})^2 + 2\nabla \phi_{\text{ex}} \cdot \nabla \phi_q] ds \\ &= -K \int_V \delta\phi_q \nabla^2 \phi_{\text{ex}} d\mathbf{r} + K \int_{\partial V} \boldsymbol{\sigma} \cdot \{\nabla \phi_{\text{ex}} \delta\phi_q + \tfrac{1}{2} \delta\mathbf{q} [(\nabla \phi_{\text{ex}})^2 + 2\nabla \phi_{\text{ex}} \cdot \nabla \phi_q]\} ds, \end{aligned} \tag{14}$$

where the boundary ∂V is the ''surface'' of the disclination core and σ is a unit vector normal to ∂V.

We can use the diffusion equation for the field outside of the core regions to write Eq. (11) in a frame-invariant manner as

$$\int_V \delta\phi D\nabla^2 \phi d\mathbf{r} = -\frac{1}{\gamma_1} \delta\mathcal{F}, \tag{15}$$

which, in terms of ϕ_q and ϕ_{ex}, is

$$\int_V \delta\phi_q [-\dot{\mathbf{q}} \cdot \nabla \phi_q + D\nabla^2 \phi_{\text{ex}}] d\mathbf{r} = -\frac{1}{\gamma_1} \delta\mathcal{F}. \tag{16}$$

Combining Eqs. (13), (14), and (16) gives the equation of motion for $\mathbf{q}$:

$$\tilde{\boldsymbol{\eta}} \cdot \dot{\mathbf{q}} = D \int_{\partial V} \left\{ \nabla \phi_q (\mathbf{f} \cdot \sigma) - \frac{\sigma}{2} [\mathbf{f}^2 + 2\mathbf{f} \cdot \nabla \phi_q] \right\} ds, \tag{17}$$

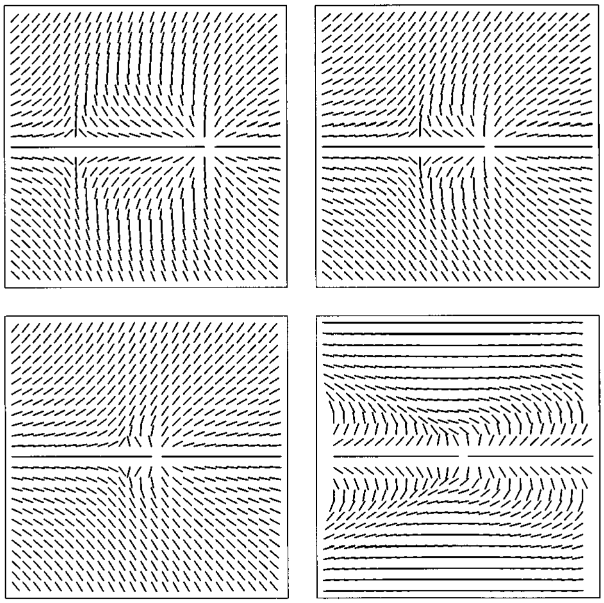

FIG. 1. Director field for disclination-antidisclination pair annihilating shown at times $t=0$, 70, 95, and 101.3.

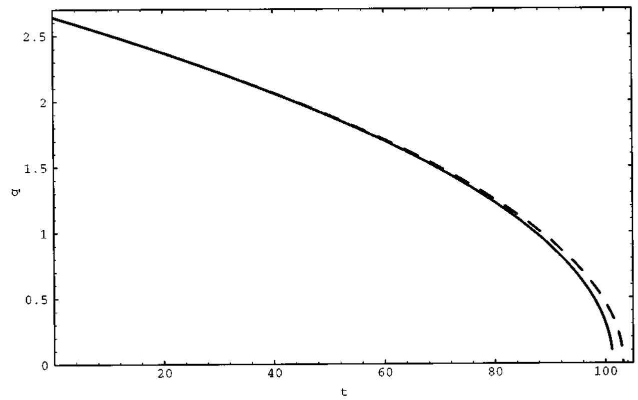

FIG. 2. Position vs time for the disclination-antidisclination pair annihilation shown in Fig. 1.

where $\mathbf{f}=\nabla\phi_{\mathrm{ex}}|_q$ and $\widetilde{\boldsymbol{\eta}}=\int_V \nabla\phi_q \nabla\phi_q d\mathbf{r}$ is a 2×2 matrix, not a scalar. For a small external field gradient at $\mathbf{x}=\mathbf{q}$ and small core radius, we can take $\mathbf{f}=\nabla\phi_{\mathrm{ex}}$ to be constant over the region of the disclination core. Neglecting terms of order $\mathbf{f}^2$, Eq. (17) becomes

$$\begin{aligned}\widetilde{\boldsymbol{\eta}}\cdot\dot{\mathbf{q}} &= D\int_{\partial V}[\nabla\phi_q(\sigma\cdot\mathbf{f})-\sigma(\mathbf{f}\cdot\nabla\phi_q)]ds\\ &= D\mathbf{f}\wedge\int_{\partial V}\nabla\phi_q\wedge\sigma ds\\ &= -2\pi s D(J\mathbf{f}),\end{aligned} \tag{18}$$

where we have used the boundary conditions, Eq. (9), in the last step, and

$$J=\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}. \tag{19}$$

The expression $\widetilde{\eta}=\int_V \nabla\phi_q\nabla\phi_q d\mathbf{r}$ can be evaluated using the explicit solution for ϕ_q given in Eq. (10). Taking the gradient of ϕ_q in Eq. (10) gives

$$\nabla\phi_q = J(\nabla g+\dot{\mathbf{q}}g/D). \tag{20}$$

After a small amount of algebra, one finds that $\dot{\mathbf{q}}$ is an eigenvector of $\widetilde{\eta}$ with eigenvalue

$$\begin{aligned}\eta &= \pi s^2\int_{\mathcal{E}}^{\infty}K_1^2(\mu)I_1(2\mu)d\mu\\ &\approx \pi s^2\ln[3.7D/(|\dot{\mathbf{q}}|a)],\end{aligned} \tag{21}$$

where $\mathcal{E}=a|\dot{\mathbf{q}}|/(2D)$, and a is the core radius. This is the same friction coefficient found in Ref. 10. So our equation of motion becomes

$$\eta\dot{\mathbf{q}} = -2\pi s D(J\mathbf{f}). \tag{22}$$

Note that in the case where $\mathbf{f}=\nabla\phi_{\mathrm{ex}}|_q$ is not small, one must use the more exact Eq. (17).

As an example of the use of the equation of motion (22), let us consider the annihilation of a pair of disclinations with opposite winding numbers. The importance of this example lies in the fact that there is growing numerical evidence[19,20] that the phase ordering of a large system of numerous defects is determined solely by the forces acting in the two-defect problem. We place a disclination with $+s$ at $x=-q$ on the x axis and one with $-s$ at $x=q$. The field ϕ, can be found by using Eq. (10) twice with a suitably shifted origin. We find the equation of motion for the disclination at $x=q$ and assume that the other follows in a symmetric fashion. The gradient caused by the positive disclination at the site of the second is

$$\nabla\phi_+|_{x=q} = \frac{s|\dot{q}|}{2D}\exp\left(\frac{-q\dot{q}}{D}\right)\left[K_1\left(\frac{q|\dot{q}|}{D}\right)-K_0\left(\frac{q|\dot{q}|}{D}\right)\right]\hat{\mathbf{y}}. \tag{23}$$

Substituting this into Eq. (22) gives the equation of motion for q. The resulting equation is extremely nonlinear and cannot be solved analytically for $\dot{q}$ in terms of q. The problem can be simplified greatly from a numerical point of view by differentiating the equation of motion with respect to time and converting to a first-order system of two equations. The original equation of motion supplies a constraint on the choice of initial conditions for q and $\dot{q}$. The resulting system is

$$\begin{aligned}\dot{q} &= y,\\ \dot{y} &= \frac{\dot{q}^2}{q}\frac{K_1(q|\dot{q}|/D)}{\mathcal{E}K_1^2(\mathcal{E})I_1(2\mathcal{E})\exp(-q\dot{q}/D)-K_1(q|\dot{q}|/D)}.\end{aligned} \tag{24}$$

Note that $\mathcal{E}$ depends on $\dot{q}$ from Eq. (21). Despite the complicated nature of these equations it is considerably simpler to solve these ordinary differential equations than to solve the full partial differential equations describing the fields. These equations have an approximate scaling solution for small t of

$$q = cD^{1/2}(t_d-t)^{1/2}, \tag{25}$$

where c comes from numerically solving the equation of motion at $t=0$ given t_d, an annihilation time. Figure 1 displays a field map of the numerical solution to Eqs. (24) at different times. A comparison of the numerical solution and Eq. (25) is given in Fig. 2. Note that the scaling solution remains almost indistinguishable from the numerical solution until quite close to the annihilation time t_d.

Another interesting implication of the dynamic equations of motion is that a finite flow is required to move a disclination in a finite medium. In the static case, the position of a disclination is fixed by the boundaries. This is due to the fact that the gradient of ϕ caused by a static disclination drops off only as $1/r$ at large distances r from the disclination. In addition, the line tension σ, computed using the energy in Eq. (3), diverges logarithmically with system size, $\sigma_s=\pi K s^2 \ln(L/a)$. L is the distance of the disclination line from the walls of the container.[6] In contrast, if one examines the field in Eq. (10) due to a disclination that is moving, one finds that it drops to zero at distances much greater than $a/\mathcal{E}$. The *dynamic* line tension, computed using the solution (10) in Eq. (3), is given by

$$\sigma=\pi K s^2\int_{\mathcal{E}}^{\infty} d\mu\,\mu\{I_0(2\mu)[K_0^2(\mu)+K_1^2(\mu)] + 2I_1(2\mu)K_0(\mu)K_1(\mu)\} \approx \pi K s^2 \ln(1.12/\mathcal{E}), \tag{26}$$

where $\mathcal{E}$ is the same as in Eq. (21). We can see from this that the static and dynamic line tensions are equal when $1/\mathcal{E}\approx L/a$ or when the speed of the flow is $|\dot{\mathbf{q}}|=2K/(\gamma_1 L)$. For flow speed less than this critical value, the disclination will be pinned elastically by the boundaries. Above the critical flow speed, the field distortions due to the disclination do not reach the boundary, and the disclination is free to move.

In conclusion, in this paper we have derived an equation of motion for a disclination in a nematic liquid crystal. This equation has no logarithmic dependence on the system size. We have applied this equation to the annihilation of a pair of opposite-strength disclinations and the flow required to free a disclination from the walls of its container. An observation of these two effects would give an experimental measurement of the ratio of the elastic constant to the viscosity constant. We note, however, that these results depend on the assumption that the dissipation inside the core is negligible compared to that outside the core. This will only occur when the size of the region outside the core where the dissipation is significant is much greater than the core itself or $\mathcal{E}\ll 1$.

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