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Fluctuations of topological disclination lines in nematic liquid crystals: Renormalization of the string model

D. Svenšek* and S. Žumer
Department of Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia
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Using the tensorial Landau–de Gennes theory, we study the fluctuations of a disclination line in a nematic liquid crystal. By analyzing the structure and the spectrum of the eigenmodes of a line of strength $\pm 1/2$, we reassess the concept of line tension used in the simple string model of the disclination showing that it does not include the complete set of eigenmodes and must be renormalized. In general, the line tension considerably underestimates the thermal amplitude of a disclination and we find that it is only applicable to severely confined disclinations.

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As a signature of orientational order, topological defects are very important for identification, experimental studies, and applications of liquid crystals [1]. Since the early days of liquid-crystalline science, the range of techniques has been extended from passive observation of static structures by polarization microscopy to preparation and manipulation of defect structures and detailed analysis of motion, annihilation, and thermal fluctuations of defects [2–6]. The motivation for these experiments transcends purely scientific curiosity: for example, defect dynamics is crucial for switching in nematic bistable devices [7,8] or multidomain cells [9].

A considerable part of the experiments remains poorly understood. While it is now widely accepted that the structure of the defects is rather nontrivial—for example, the core of an $s=1/2$ disclination line consists of a uniaxial nematic phase surrounded by a biaxial mantle (Fig. 1) [10]—the associated fluctuation dynamics has only been studied within the director description [11,12]. In this paper, we analyze the fluctuation eigenmodes at a straight $s=\pm 1/2$ disclination line using the full tensorial framework. We focus on the soft modes that correspond to the string fluctuations, and we challenge and delimit the validity of the simple string model of the disclination [13] thereby establishing contact with experimental observables such as its thermal amplitude or kinematics in general. We also extrapolate our main results to disclination lines in smectic-*C* liquid crystals and vortex lines in superfluids. String models of a line defect are encountered in various areas of physics, yet with different levels of approximation. In this paper, we present a rare example where the degree of validity of the model can be determined exactly.

We start with Landau–de Gennes free energy density. In the one-constant approximation, it consists of three bulk terms and a single elastic term,

$$f = \frac{1}{2}A\ \mathrm{Tr}\mathsf{Q}^2 + \frac{1}{3}B\ \mathrm{Tr}\mathsf{Q}^3 + \frac{1}{4}C(\mathrm{Tr}\mathsf{Q}^2)^2 + \frac{1}{2}L\ \mathrm{Tr}(\nabla\mathsf{Q}\cdot\nabla\mathsf{Q}), \tag{1}$$

and is invariant upon a homogeneous rotation of the Q tensor. In the cylindrical coordinate system $\{\hat{\mathbf{e}}_r,\hat{\mathbf{e}}_\phi,\hat{\mathbf{e}}_z\}$ with $\hat{\mathbf{e}}_z$ along the disclination core, the eigensystem of the order parameter tensor rotates as $\psi=\psi_0+(s-1)\phi$ with respect to the above base vectors when we encircle a defect of strength *s* at the origin (Fig. 1); ψ is the angle between $\hat{\mathbf{e}}_r$ and the director in the far field, and $\psi_0=\psi(\phi=0)$.There is no dependence on ϕ other than this rotation, i.e., the scalar invariants of Q (the degrees of order and biaxiality) are ϕ independent.

If we define another triad $\{\hat{\mathbf{e}}_1,\hat{\mathbf{e}}_2,\hat{\mathbf{e}}_z\}$ such that $\hat{\mathbf{e}}_1=\hat{\mathbf{e}}_r\cos\psi+\hat{\mathbf{e}}_\phi\sin\psi$ and $\hat{\mathbf{e}}_2=-\hat{\mathbf{e}}_r\sin\psi+\hat{\mathbf{e}}_\phi\cos\psi$, the Q eigensystem of the ground state coincides with this triad everywhere. Introducing the orthonormal symmetric traceless base tensors [14]: $\mathsf{T}_0=(3\hat{\mathbf{e}}_z\otimes\hat{\mathbf{e}}_z-\mathsf{I})/\sqrt{6}$, $\mathsf{T}_1=(\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_1-\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_2)/\sqrt{2}$, $\mathsf{T}_{-1}=(\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_2+\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_1)/\sqrt{2}$, $\mathsf{T}_2=(\hat{\mathbf{e}}_z\otimes\hat{\mathbf{e}}_1+\hat{\mathbf{e}}_1\otimes\hat{\mathbf{e}}_z)/\sqrt{2}$, $\mathsf{T}_{-2}=(\hat{\mathbf{e}}_z\otimes\hat{\mathbf{e}}_2+\hat{\mathbf{e}}_2\otimes\hat{\mathbf{e}}_z)/\sqrt{2}$, the ground state Q tensor components are ϕ independent, while the components of an arbitrary perturbation can be rotated around $\hat{\mathbf{e}}_z$ at no cost. Hence the dependence of the eigenmode components on ϕ is sinusoidal. Similarly, the ground state is *z* independent and the dependence of the eigenmode components on *z* is sinusoidal.

We first look for the Goldstone modes, as they yield families of slowly relaxing and spatially extensive "soft" fluctuation modes that can be easily observed. "Massive" fluctuations are less interesting, as they are shortlived ($\approx$100 ns) and localized ($\approx$10 nm). Besides the homogeneous rotations of the Q tensor, which in a deformed nematic are soft only in the one-constant approximation, in a deformed system there

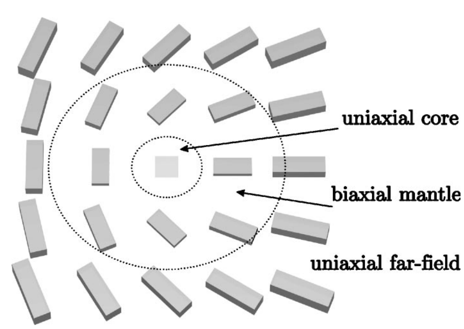

FIG. 1. Tensorial core structure of the $1/2$ disclination. The Q tensor eigensystem is represented by the orientation of the box, lengths of the edges are a measure of the eigenvalues.

*Author to whom correspondence should be addressed. FAX: +386 1 2517281. Email address: daniel@fiz.uni-lj.si

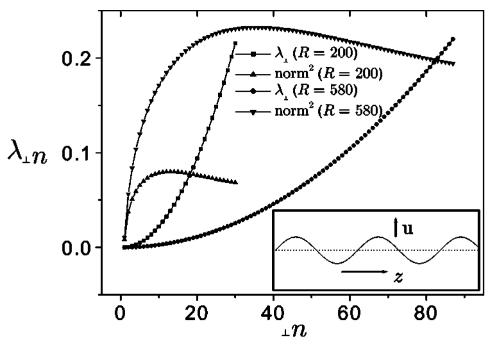

FIG. 2. Radial eigenvalue $\lambda_{\perp n}$ (in units of $1/\tau$) and the norm squared (arbitrary units) of the nth radial eigenfunctions for two radii of confinement. For $R=200$, $\lambda_{\perp 1}=1.4\times 10^{-5}$, $\lambda_{\perp 2}=4.5\times 10^{-4}$, $\lambda_{\perp 3}=1.4\times 10^{-3}$; note that $\lambda_{\perp 2}/\lambda_{\perp 1}\approx 30$. Inset: the string fluctuation of the disclination line.

exist nontrivial Goldstone modes not subject to this approximation, corresponding to homogeneous displacement of the structure—in our case displacement of the disclination line. Since translational degrees of freedom are absent in this analysis, displacement is achieved by modifying the order parameter field. Modulating the displacement modes sinusoidally along $\hat{\mathbf{e}}_z$ results in the string fluctuations of the disclination line (Fig. 2, inset).

Setting $\mathsf{Q}(\mathbf{r},t)=q_i(\mathbf{r},t)\mathsf{T}_i(\mathbf{r})$, the elastic part of (1) is

$$f^e=\frac{L}{2}\left\{\sum_i\left[\left(\frac{\partial q_i}{\partial r}\right)^2+\left(\frac{\partial q_i}{\partial z}\right)^2\right]+\frac{1}{r^2}\left[\left(\frac{\partial q_0}{\partial\phi}\right)^2+\left(\frac{\partial q_1}{\partial\phi}-2s\;q_{-1}\right)^2+\left(\frac{\partial q_{-1}}{\partial\phi}+2s\;q_1\right)^2+\left(\frac{\partial q_2}{\partial\phi}-s\;q_{-2}\right)^2+\left(\frac{\partial q_{-2}}{\partial\phi}+s\;q_2\right)^2\right]\right\},\quad(2)$$

while the bulk part of (1) is a polynomial in q_i. We introduce dimensionless quantities $r\leftarrow r/\xi$, $t\leftarrow t/\tau$, $(A,B,C)\leftarrow(A,B,C)\xi^2/L$, where ξ is the correlation length, typically a few nanometers, and $\tau=\mu_1\xi^2/L$ is the characteristic time, typically tens of nanoseconds; here μ_1 is the "bare" rotational viscosity [15]. Neglecting the hydrodynamic flow, the order parameter dynamics is governed by the time-dependent Ginzburg-Landau equation

$$\frac{\partial q_i}{\partial t}=\nabla\cdot\frac{\partial f}{\partial\nabla q_i}-\frac{\partial f}{\partial q_i}.\quad(3)$$

The ground state involves only components along T_0 and T_1, $\mathsf{Q}_0(\mathbf{r})=a_0(r)\mathsf{T}_0+a_1(r)\mathsf{T}_1$, whereas fluctuations include all five components: $\Delta\mathsf{Q}(\mathbf{r},t)=x_i(\mathbf{r},t)\mathsf{T}_i$. The fluctuation eigenmodes x_i, satisfying $\dot{x}_i=-\lambda x_i$, are sought by the *Ansätze*

$$x_i=R_{i,m}(r)\Phi_i(m\phi)\sin(kz)\exp(-\lambda t),\quad i=0,\pm 1\quad(4)$$

$$x_i=R_{i,m'}(r)\Phi_i(m'\phi)\sin(kz)\exp(-\lambda t),\quad i=\pm 2\quad(5)$$

where $\Phi_i(x)=\cos x$ for $i\geqslant 0$ and $\Phi_i(x)=\sin x$ for $i<0$; the global angular phase and the z phase are arbitrary. Due to the continuity and differentiability requirements, m is an integer, whereas m' is a half-integer. In the one-constant approximation, the two sets of components x_i [Eq. (4) and (5)] are not coupled, i.e., in-plane ($i=0,\pm 1$) and out-of-plane ($i=\pm 2$) fluctuations are independent. Furthermore, the z dependence is fully decoupled: the radial eigenfunctions $R_i(r)$ do not depend on k and the cross-section structure of the disclination line is not affected by the modulation along z.

We focus on the in-plane fluctuations. Setting the *Ansatz* into Eq. (3), we obtain the eigensystem for the radial functions $R_{i,m}(r)$

$$\nabla^2R_{0,m}+\left(\lambda_\perp-g_0(r)-\frac{m^2}{r^2}\right)R_{0,m}+g_{01}(r)R_{1,m}=0,\quad(6)$$

$$\nabla^2R_{1,m}+\left(\lambda_\perp-g_1(r)-\frac{m^2+4s^2}{r^2}\right)R_{1,m}-\frac{4sm}{r^2}R_{-1,m}+g_{01}(r)R_{0,m}=0,\quad(7)$$

$$\nabla^2R_{-1,m}+\left(\lambda_\perp-g_{-1}(r)-\frac{m^2+4s^2}{r^2}\right)R_{-1,m}-\frac{4sm}{r^2}R_{1,m}=0,\quad(8)$$

where $\lambda=\lambda_\perp+k^2$ and $\lambda_\perp$ is the eigenvalue of the radial and angular part, whereas g_i are quadratic polynomials of the ground state components. Note that defects of strengths s and $-s$ are formally equivalent, as changing the sign of the defect and redefining $\mathsf{T}_{-1}\rightarrow-\mathsf{T}_{-1}$ and $\mathsf{T}_{-2}\rightarrow-\mathsf{T}_{-2}$ preserves the sign of s in the equations. In our case $s=1/2$, though it can be any (half-)integer in principle.

For an infinite system, one can determine the homogeneous displacement mode directly by construction. It corresponds to $\lambda_\perp=0$ (no energy cost) and $m=1$ (displacement has dipolar symmetry). Setting $\mathsf{Q}_0(\mathbf{r}-\mathbf{u})=\mathsf{Q}_0(\mathbf{r})+\Delta\mathsf{Q}(\mathbf{r})$, the perturbation $\Delta\mathsf{Q}$ corresponding to the displacement $\mathbf{u}$ is $\Delta\mathsf{Q}(\mathbf{r})=-\mathbf{u}\cdot\partial\mathsf{Q}_0/\partial\mathbf{r}$, which reads

$$x_0(\mathbf{r})\mathsf{T}_0+x_1(\mathbf{r})\mathsf{T}_1+x_{-1}(\mathbf{r})\mathsf{T}_{-1}=-\mathbf{u}\cdot\left(\hat{\mathbf{e}}_r\frac{\partial a_0}{\partial r}\mathsf{T}_0+\hat{\mathbf{e}}_r\frac{\partial a_1}{\partial r}\mathsf{T}_1+\hat{\mathbf{e}}_\phi\,2s\frac{a_1}{r}\mathsf{T}_{-1}\right).\quad(9)$$

The lowest family of string modes is generated by adding the z dependence. Hence $\lambda=k^2$, or $\lambda=Lk^2/\mu_1=Kk^2/\gamma_1$ in physical units, where K is the Frank elastic constant and γ_1 is the rotational viscosity. This is an exact result for the relaxation rate of the string mode.

Let us interpret these results by comparing them with a simple picture of the disclination line. The director free energy per unit length—line tension—of a straight disclination line with strength s is

$$\mathcal{F}_0=\pi s^2K\ln\frac{R}{r_0},\quad(10)$$

where K is the Frank elastic constant, R the system size, and r_0 a microscopic cutoff determined by the core energy. Hence, in a model the disclination line can be considered as a simple string under tension [13]. The energy cost of its (overdamped) fluctuation modes (Fig. 2, inset), which can be attributed to the increase in length, $\Delta l = \int dz (\partial u/\partial z)^2/2$, is thus $\Delta F = \frac{1}{2}k^2 u^2 \mathcal{F}_0 \int dz\, \cos^2 kz$, where u is the amplitude and k the wave vector of the mode.

In the complete description, the energy cost of any fluctuation eigenmode $\mathbf{x}$ is given by $\Delta F(\mathbf{x}) = \lambda \int dV x_i^2/2$. For the homogeneous displacement mode (9) this reads

$$\Delta F = \frac{1}{2}k^2 u^2 \underbrace{\pi \int r dr \left[\left(\frac{\partial a_0}{\partial r}\right)^2 + \left(\frac{\partial a_1}{\partial r}\right)^2 + 4s^2 \left(\frac{a_1}{r}\right)^2 \right]}_{\mathcal{F}_0'} \times \int dz\, \cos^2 kz. \tag{11}$$

Comparing Eq. (11) (multiplied by $L\xi$ to revert to physical units) with the form of the energy cost of the simple string fluctuation, a line tension can be defined for the disclination line as indicated by the underbrace. If the string model were accurate, the line tension $\mathcal{F}_0'$ would be the actual free energy (1) of the unperturbed disclination line per unit length. But it is exactly the elastic free energy [Eq. (2)] per unit length, whereas the bulk contributions are absent, indicating that the volume of the disclination core is unaffected by the fluctuations. Only the elastic terms contribute to the line tension. It must be stressed that within the isotropic order parameter elasticity this finding is universal. Far from the defect core where the bulk free energy contributions vanish, the string model is correct. Moreover, using the bulk values of a_0 and a_1, the line tension (10) is recovered exactly. However, it must be emphasized that due to the director distortion this regime is not approached exponentially but by a power law.

Let us now concentrate on the $m=1$ fluctuations with $\lambda_\perp > 0$. In solving Eqs. (6)–(8), we confine the system at a radius R with the restriction $R_{i,m,n}(R)=0$ in order to get a discrete spectrum $\lambda_{\perp n}$. One might argue that this boundary condition is rather unphysical. In a real sample, however, one never deals with an ideally isolated disclination line—it is surrounded by other defects and irregularities. The boundary condition should therefore be viewed as an effective confinement. In the limit $R \to \infty$, physical observables should be only weakly dependent of R, such as the free energy (10). Furthermore, if one uses the boundary condition $R'_{i,1,n}(R) = 0$, the lowest eigenmode is of the growing type, with $\lambda_{\perp 1} \propto 1/R^2 < 0$, reflecting the instability of the disclination towards the escape from the system. This finite-size effect is often manifest in experimental situations: defects are attracted to the boundary or even pass through it if the anchoring is weak enough.

The boundary conditions at $r=0$ are obtained by finding the analytic behavior of the ground state and the perturbations for small r. The eigensystem (6)–(8) is discretized and efficiently solved by a multidimensional Newton relaxation method [16], Fig. 3. In the physically relevant limit $R \gg \xi$, the radial dependence of the lowest modes for $r \ll R$ is given by Eq. (9): Each of these modes contributes to the displacement $\mathbf{u}$ of the central part. Still in the limit $R \gg \xi$, the difference $\sqrt{\lambda_{\perp n+1}} - \sqrt{\lambda_{\perp n}}$ approaches π/R as $n \to \infty$, i.e., $\lambda_{\perp n} \to (\text{const} + n\pi/R)^2$, Fig. 2. For $n \gg 1$, the eigenvalue of the nth mode scales as $\lambda_{\perp n} \propto 1/R^2$.

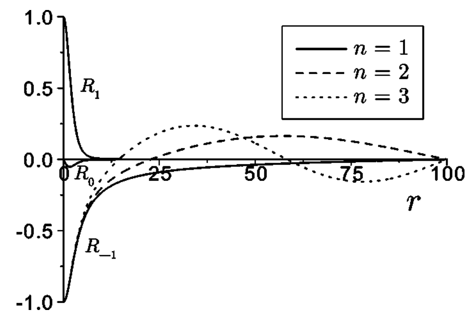

FIG. 3. Three lowest radial eigenfunctions (not normalized) for $m=1$. For $i=0,1$ the functions $R'_{i,m,n}$ overlap on the scale of the graph.

We have shown that the simple string model only includes the lowest $m=1$ fluctuation mode. Thus, quite universally, the contributions of the higher $m=1$ modes represent a renormalization of the model. Thermal fluctuation amplitude of the kth Fourier component at $r=0$ is

$$\langle \Delta Q_i^2(r=0, m=1, k)\rangle = 2\sum_n \langle c_{k,n}^2\rangle R_{i,1,n}^2(0), \tag{12}$$

where $R_{i,1,n}$ are normalized and $\langle c_{k,n}^2\rangle = k_B T / L\xi(k^2 + \lambda_{\perp n})$ given by equipartition theorem; the factor of 2 comes from the twofold angular degeneracy of the modes. The displacement $\langle \mathbf{u}_k^2\rangle$ of the line is obtained from Eq. (12) by means of Eq. (9). If only the lowest radial mode is taken into account in Eq. (12), which is equivalent to using the nonrenormalized string model, the thermal amplitude is obviously underestimated (Fig. 4) or conversely, the extracted value of K is too low. The error increases rather slowly (logarithmically) with R; for experimentally relevant length scales it is of the order of 100%. The failure of the string model is best demonstrated in the limit $R \to \infty$: for a fixed and nonzero k, $\langle \mathbf{u}_k^2\rangle \to 0$ if only the lowest radial mode is taken into account, since the norm squared of the mode logarithmically diverges for $R \to \infty$. Alternatively, the same can be seen by noting the logarithmic divergence of the line tension (10).

To simulate or analyze a real observation of the disclination line fluctuations, for a given k, one has to sum up a proper number of radial modes possessing a considerable thermal amplitude. The maximum number is set by the resolution of the instrument—the summation should be stopped at the latest when the first zero of the radial functions becomes comparable to the resolution. As in a real situation $1/k$ is large compared to the resolution, the series is always truncated earlier by the diminishing thermal amplitude and hence there is no cutoff ambiguity. The two characteristic regimes are illustrated in Fig. 4: if $\pi/k \ll R$, many radial modes have to be summed up and the fluctuation amplitude is essentially independent of the system size R (upper diagram); if $\pi/k \gg R$ (severe confinement) a few modes suffice and the fluctuation amplitude is suppressed by decreasing R (lower diagram).

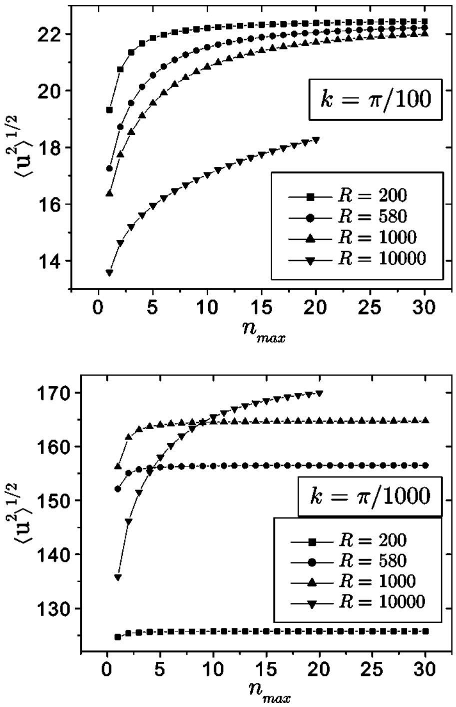

FIG. 4. rms displacement of the disclination line (the length unit is ξ) vs the number of radial modes summed in the regimes of weak (upper diagram) and severe confinement; $n_{max}=1$ corresponds to the nonrenormalized string model. The maximum size of the computational domain is $R=580$, the values beyond this range ($R=1000$, $R=10\,000$) are extrapolated.

Of course, there exist other soft fluctuation modes which have not been discussed here. They are either zero at $r=0$ or involve out-of-plane components, and thus these modes are not important for the fluctuations of the disclination line. For example, the $m=0$ soft mode, which involves only the component x_{-1} [in this case Eq. (8) is decoupled], corresponds to the Goldstone rotation of Q around the z axis. Naturally, it is present regardless of the configuration; the defect structure merely causes the radial eigenfunction to decay at the uniaxial core.

In summary, we have demonstrated that the simple string model of the disclination line is generally inadequate, and we have shown how the amplitude of line fluctuations can be calculated consistently within the tensorial formalism. Our results are valid in the approximation where the gradients along z enter the free energy in purely quadratic terms, which holds not only for nematic liquid crystals but also for smetic-C liquid crystals in the one-constant approximation as well as for superfluids. Superconductors and their analogues smectic-A liquid crystals [17] possess an additional vector order parameter (vector potential **A**/nematic director) besides the XY-model degrees of freedom $\Psi=|\Psi|\exp(i\phi)$ (superconducting wave function/smectic density wave). Here $\nabla\Psi$ and **A** are coupled by $|(-i\hbar\nabla-e\mathbf{A})\Psi|^2/2m$, which implies that gradients along z induce a change in **A**. As a consequence, fluctuations of a vortex line in superconductors or a dislocation in smectic-A liquid crystals cannot be reduced to mere displacements but also include distortions of the line structure. Thus the actual line tension cannot be consistently interpreted as the free energy per unit length, not even asymptotically. However, one can still define an effective line tension using a string model renormalized by the higher radial modes.

Backflow has been neglected in this study. One expects that it will have mainly an advective effect, causing translational motion of the line on top of director rotation. Considering the symmetry breaking caused by backflow in the case of pair annihilation [18], we expect the relaxation rate λ to increase due to backflow, at least for the $+1/2$ line. The increase might be of order of 100% and is expected to decrease with increasing wave vector k as the shearing gets stronger.

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