Invited lecture/Scientific contribution

Altering the Position of Topological Defects in Nematic Shells

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Abstract:
Topological defects (TDs) in liquid crystals may have their locations experimentally altered by locally distorting the liquid crystalline (LC) order, e.g., by the melting induced by optical tweezers. In this research, we investigated the nematic ordering profiles and accompanying topological defect configurations in thin nematic liquid crystalline shells that are subject to externally forced local LC order distortions. We show that inside curved LC films these manipulations are greatly influenced by local Gaussian curvature if it displays strong spatial variability. We use a mesoscopic model in which the curvature of the surface and the nematic order parameter tensor serve to explain the shell geometry and LC orientational order. We demonstrate that TDs are rather tightly "glued" to a local Gaussian curvature on increasing the prolateness of shells.

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1. Introduction

Localized deformations in a physical field known as topological defects (TDs) are protected by topology (Mermin, 1979) and are of interest to all branches of physics due to their interdisciplinary nature (Zurek, 1985). The topological charge of TDs is their essential property, which is conserved (Mermin, 1979; Volovik, et al. 1983), thus governing transformations between different defect arrangements, such as merging and splitting (Svenšek, et al. 2004; Kralj, et al. 2017). Nematic liquid crystalline (LC) shells provide an ideal platform for studying the impact of topology and geometry on TDs (Nelson, 2002; Vitelli, et al. 2006; Skačej, et al. 2008; Lopez-Leon, et al. 2011; Rosso, et al. 2012). These shells are composed of thin nematic films that cover micrometer-sized colloidal objects and have a typical molecular length thickness.

Anisotropic LC molecules, such as rod-like molecules, form the basis of the simplest nematic LCs (Kleman, et al. 2003). These materials have both liquid-like properties and orientational order, which is described at the mesoscopic level by the nematic director field $\vec{\boldsymbol{n}}$, indicating the average molecular direction in the local region. Nematic shells are effectively two-dimensional (2D) systems, with the $\vec{\boldsymbol{n}}$ orientations confined within a curved 2D film (Nelson, 2002), which generally results in the domination of topological defects (TDs) in such structures.

Topological defects (TDs) in 2D nematic films are identified by their winding number $\boldsymbol{m}$, which can take on half-integer values due to the $\pm\vec{\boldsymbol{n}}$ invariance. This number describes the number of rotations of $\vec{\boldsymbol{n}}$ on encircling by any path the defect center counterclockwise. Defects with positive and negative values of $\boldsymbol{m}$ are referred to as defects and antidefects, respectively (Poincaré, 1886; Kamien, 2002).

Softness (strong responsivity to local stimuli) is a crucial feature of liquid crystals. Researchers have demonstrated that nematic TDs can be efficiently manipulated using laser beams (Nych, et al. 2017; Tkalec, et al. 2011; Liu, et al. 2013; Smalyukh, 2020), as the beam can locally melt the orientational order. Since orientational order is melted also within the core of defects, it is advantageous for TDs to be assembled within regions where the nematic order is reduced, as the penalty for forming the defect core is reduced. However, we demonstrate in this work that on effectively two-dimensional curved surfaces, the manipulation of nematic TD positions by laser beams is limited as TDs are relatively strongly attached to a local Gaussian curvature.

2. Methods

We utilize mesoscopic modeling to characterize the shapes of two-dimensional curved surfaces and the nematic ordering within them, employing the curvature tensor $\underline{C}$ and the nematic order tensor Q to describe the system's properties (Rosso, et al. 2012). The Weingarten curvature tensor $\underline{C}$ determines the local surface curvature:

$$\underline{C} = C_1 \ \vec{e_1} \ \otimes \vec{e_1} + C_2 \vec{e_2} \otimes \vec{e_2} \ , \tag{1}$$

where the unit vectors $\{ \vec{e_1}, \vec{e_2}\}$ are oriented along the surface principal directions exhibiting principal curvatures $\{C_1, C_2\}$. The local mean curvature H and the Gaussian curvature K can be calculated as:

$$H \coloneqq \frac{Tr[\underline{C}]}{2} = \frac{C_1+C_2}{2}, \ K \coloneqq Det[\underline{C}] = C_1 C_2. \tag{2}$$

The local nematic orientational order on the surface is characterized by the two-dimensional tensor order parameter $\underline{Q}$ (Kralj, et al. 2011). The molecules exhibiting orientational ordering are required to lie in the local tangent plane of the surface but are otherwise unrestricted. We assume rod-like molecules with head-to-tail invariance. Tensor $\underline{Q}$ can be represented in diagonal form as follows (Kralj, et al. 2011):

$$\underline{Q} = \lambda(\vec{n} \otimes \vec{n} - \vec{n}_\perp \otimes \vec{n}_\perp), \tag{3}$$

where $\vec{n}$ and $\vec{n}_\perp$ are its unit eigenvectors, while $\lambda \in [0, 1/2]$ and $-\lambda$ are the corresponding eigenvalues. When λ is equal to zero, the system is in a locally isotropic state with no orientational order. In contrast, when λ is equal to 1/2, the system is in a locally

ordered state where the molecules are rigidly aligned in the direction of the nematic director field $\vec{n}$.

The total free energy functional of the LC shell surface is given by $F = \iint f \mathrm{d}^2 r$, where the free energy density $f = f_c + f_e$ is the sum of the order condensation (f_c) and elastic (f_e) terms (Kralj, et al. 2011; Mesarec, et al. 2016). To illustrate the features of interest, we utilize a minimal model and express the nematic elasticity in terms of a single elastic constant k. The energy densities are expressed as

$$f_c = -\alpha Tr Q^2 + \beta (Tr Q^2)^2, \tag{4a}$$

$$f_e = k \mathrm{Tr}((\nabla_s Q)^2). \tag{4b}$$

Material constants α and β must take positive values to enable orientational ordering in the system. The order parameter correlation length ξ, which depends on the material properties, is defined as $\xi = \sqrt{k/|\alpha|}$. This parameter estimates the distance at which a local perturbation in the order parameter relaxes on a flat surface. We introduce R as the radius of the sphere with the same surface area as the surface area of the investigated shell. The bulk equilibrium value of the order parameter in flat geometries is $\lambda_0 = \sqrt{\alpha/\beta}/2$.
To model the laser beam, we implemented a boundary condition that locally melts the orientational order. We enforce the melting process by setting $\lambda = 0$ at certain points, while calculating the orientational ordering by minimizing the total free energy at all other points.

3. Results

We are studying how to manipulate topological defects (TDs) in nematic shells using laser-induced local distortions, which cause the nematic order to melt locally (Mesarec, et al. 2022). In our simulations, we simulate these distortions by varying the position of a melted region within prolate shells. It is well-established that local melting attracts TDs in the nematic phase (Nych, et al. 2017; Tkalec, et al. 2011; Liu, et al. 2013; Smalyukh, 2020), as both melting and TDs introduce a strong energy penalty. Since the core of a TD is essentially melted, the total energy penalty is generally reduced when the melted region and TD are in the same location. Therefore, we refer to a melted region as a distortion.
We are examining prolate shells that have a distinct spatial dependency in their Gaussian curvature (Mesarec, et al. 2022). On such shells, topological defects (TDs) tend to be closely situated near the poles where Gaussian curvature has the highest value. In Figure 1a, we show that in the absence of distortion, TDs are found close to the poles. When a distortion is introduced near the lower pole, as shown in Figure 1b, we can observe manipulation of the relative position of the TDs in the lower part of the prolate shell. One TD remains fixed within the distortion while the other shifts based on the interaction between the defects and the local Gaussian curvature. The positions of the remaining two TDs remain unchanged, indicating that their placement is mainly influenced by the local Gaussian curvature and their mutual elastic repulsion (Mesarec, et al. 2022). Similar phenomenon occurs in Figure 1c, where a distortion is again introduced near the region with high Gaussian curvature but slightly higher than in Figure 1b. If the distortion is moved outside of the area where the Gaussian curvature is high, the trapped defect is released and the defect configuration preferred by the Gaussian curvature is restored, as shown in Figure 1d. In this case, the distortion does not contain a topological defect (Mesarec, et al. 2022).

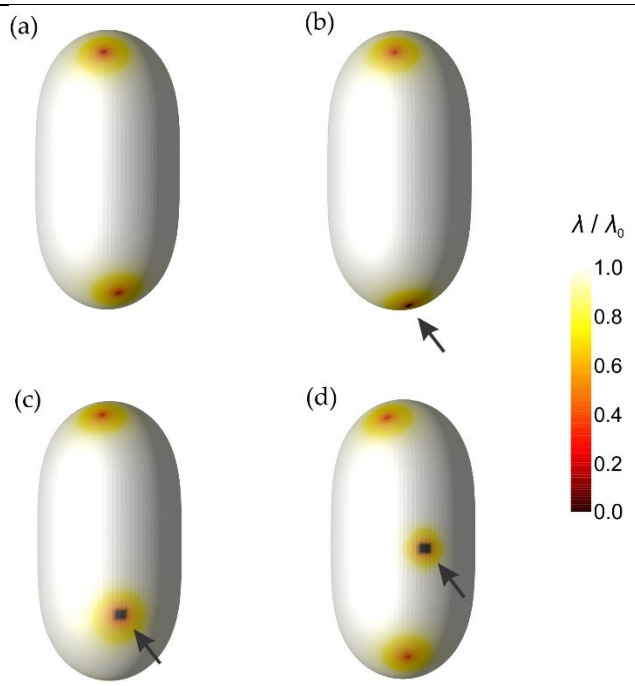

Figure 1. Equilibrium nematic ordering configurations on a prolate shell. Case without the laser beam (distortion) is presented in the panel (a), while panels (b,c,d) represent cases with different positions of the distortion (denoted by arrows). The shell shapes are presented with the superimposed nematic order parameter profiles λ. $R/\xi = 10$. Partially adapted from (Mesarec L, et al. 2022).

4. Discussion

Our study focused on manipulating TDs in nematic shells with spherical topology. We simulated the effects of introducing a localized melted region, or distortion, on the spatial distribution of TDs. Our results show that the response to distortions depends on the spatial dependence of the Gaussian curvature (Mesarec, et al. 2022). When the Gaussian curvature has a strong dependence, e.g., on prolate shape, the distortion can affect the position of TDs near poles where Gaussian curvature is high, but it cannot move TDs to the regions with low Gaussian curvature because they are strongly attracted by the regions with high Gaussian curvature. Furthermore, introducing a distortion near a certain pole on a prolate shape does not affect the TD distribution on the opposite pole (Mesarec, et al. 2022). This ability to manipulate TDs opens opportunities for various applications, such as trapping nanoparticles within their cores (Kikuchi, et al. 2002; Karatairi, et al. 2010) and forming micron-sized crystal structures (Nelson, 2002).

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References

1. Kamien RD. The geometry of soft materials: a primer. Rev. Mod. Phys. 2002; 74: 953. DOI : https://doi.org/10.1103/RevModPhys.74.953
2. Karatairi E, Rožič B, Kutnjak Z, et al. Nanoparticle-induced widening of the temperature range of liquid-crystalline blue phases. Phys Rev E Stat Nonlin Soft Matter Phys. 2010; 81: 041703. DOI: 10.1103/PhysRevE.81.041703
3. Kikuchi H, Yokota M, Hisakado Y, et al. Polymer-stabilized liquid crystal blue phases. Nature Mater. 2002; 1: 64-68. DOI: 10.1038/nmat712
4. Kleman M, Lavrentovich OD. Soft matter physics: an introduction. New York, NY: Springer New York. 2003. DOI: https://doi.org/10.1007/b97416
5. Kralj S, Rosso R, Virga EG. Curvature control of valence on nematic shells. Soft Matter. 2011; 7: 670-683. DOI: 10.1039/C0SM00378F
6. Kralj S, Murray BS, Rosenblatt C. Decomposition of strongly charged topological defects. Phys Rev E. 2017; 95: 042702. DOI: 10.1103/PhysRevE.95.042702
7. Liu Q, Senyuk B, Tasinkevych M, Smalyukh II. Nematic liquid crystal boojums with handles on colloidal handlebodies. Proceedings of the National Academy of Sciences. 2013; 110: 9231-9236. DOI: https://doi.org/10.1073/pnas.130146411
8. Lopez-Leon T, Koning V, Devaiah KBS, et al. Frustrated nematic order in spherical geometries. Nature Phys. 2011; 7: 391-394. DOI: https://doi.org/10.1038/nphys1920
9. Mermin ND. The topological theory of defects in ordered media. Reviews of Modern Physics. 1979; 51: 591. DOI: 10.1103/RevModPhys.51.591
10. Mesarec L, Góźdź W, Iglič A, Kralj S. Effective topological charge cancelation mechanism. Sci Rep. 2016; 6: 1-12. DOI: 10.1038/srep27117
11. Mesarec L, Iglič A, Kralj S. Spatial manipulation of topological defects in nematic shells. Eur Phys J E Soft Matter. 2022; 45: 62. DOI: 10.1140/epje/s10189-022-00216-z
12. Nelson DR. Toward a tetravalent chemistry of colloids. Nano Letters. 2002; 2: 1125-1129. DOI: https://doi.org/10.1021/nl0202096
13. Nych A, Fukuda JI, Ognysta U, et al. Spontaneous formation and dynamics of half-skyrmions in a chiral liquid-crystal film. Nature Physics. 2017; 13: 1215-1220. DOI: 10.1038/nphys4245
14. Poincaré H. Sur les courbes définies par les équations différentielles. J. Math. Pures. Appl. 1886; 4: 151-217. Available from: http://eudml.org/doc/234516
15. Rosso R, Virga EG, Kralj S. Parallel transport and defects on nematic shells. Continuum Mechanics and Thermodynamics. 2012; 24: 643-664. DOI: 10.1007/s00161-012-0259-4
16. Skačej G, Zannoni C. Controlling surface defect valence in colloids. Phys Rev Lett. 2008; 100: 197802. DOI: 10.1103/PhysRevLett.100.197802
17. Smalyukh II. Knots and other new topological effects in liquid crystals and colloids. Rep Prog Phys. 2020; 83: 106601. DOI: 10.1088/1361-6633/abaa39
18. Svenšek D, Žumer S. Instability modes of high-strength disclinations in nematics. Physical Review E. 2004; 70: 061707. DOI: 10.1103/PhysRevE.70.061707
19. Tkalec U, Ravnik M, Čopar S, et al. Reconfigurable knots and links in chiral nematic colloids. Science. 2011; 333: 62-65. DOI: 10.1126/science.1205705
20. Vitelli V, Nelson DR. Nematic textures in spherical shells. Phys Rev E. 2006; 74: 021711. DOI: 10.1103/PhysRevE.74.021711
21. Volovik GE, Lavrentovich OD. Topological dynamics of defects: boojums in nematic drops. Zh. Eksp. Teor. Fiz. 1983; 85: 1997-2010.
22. Zurek WH. Cosmological experiments in superfluid helium? Nature. 1985; 317: 505-508. DOI: 10.1038/317505a0