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D. Jesenek[1,2], S. Kralj[1,2,3]

CURVATURE INDUCED TOPOLOGICAL DEFECTS IN NEMATIC SHELLS

[1]Jožef Stefan Institute, Slovenia, 1000, Ljubljana, Jamova, 39
[2]Jožef Stefan International Postgraduate School, Slovenia, 1000, Ljubljana, Jamova, 39
[3]Faculty of Natural Sciences and Mathematics, University of Maribor, Slovenia, 2000, Koroška, 160
E-mail: samo.kralj@ijs.si

We study numerically impact of spatially varying curvature on position and number of topological defects (TDs). A two-dimensional Landau-de Gennes tensorial formalism is used. We focus on TDs in axially symmetric dumb-bell structures, possessing area patches exhibiting both positive and negative Gaussian curvature. These nematic shells exhibit spherical topology, enforcing the total topological charge $m_{tot}=2$. We show that on progressively narrowing necks of dumb-bell structures the number of TDs increases via nucleation of topological defect-antidefect pairs. In each surface patch, characterised by a well defined average Gaussian curvature, the sum of TDs and the total smeared Gaussian topological charge tends to be zero. Therefore, in dumb-bell structures TDs tend to spatially redistribute in a way to compensate the smeared Gaussian curvature topological charge.

Key words: *liquid crystals, nematic shells, Gaussian curvature, topological defects*

D. Jesenek[1,2], S. Kralj[1,2,3]

ТОПОЛОГИЧЕСКИЕ ДЕФЕКТЫ НЕМАТИЧЕСКИХ ОБОЛОЧЕК, ИНДУЦИРОВАННЫЕ КРИВИЗНОЙ

[1]Jožef Stefan Institute, Slovenia, 1000, Ljubljana, Jamova, 39
[2]Jožef Stefan International Postgraduate School, Slovenia, 1000, Ljubljana, Jamova, 39
[3]Faculty of Natural Sciences and Mathematics, University of Maribor, Slovenia, 2000, Koroška, 160
E-mail: samo.kralj@ijs.si

Проводится количественное изучение влияния вариации пространственной кривизны на расположение и число топологических дефектов (ТД). Использован двумерный тензорный формализм Ландау – де Жена. Внимание сосредоточено на топологических дефектах в аксиально симметричных гантелеобразных структурах, обладающих участками, проявляющими как положительную, так и отрицательную гауссову кривизну. Эти нематические поверхности (оболочки) проявляют сферическую топологию, обеспечивая общий топологический заряд $m_{общ.} = 2$. Мы показываем, что при прогрессирующем истончении «шейки» гантели возрастает число топологических дефектов, что связано с зарождением пар топологический дефект – антидефект. На каждом небольшом участке поверхности, характеризующемся хорошо выраженной гауссовой кривизной, сумма топологических дефектов и общий «размытый» гауссовый топологический заряд стремятся к нулю. Поэтому в гантелеобразных структурах топологические заряды склонны к пространственному перераспределению для компенсации «размытого» топологического заряда гауссовой кривизны.

Ключевые слова: *жидкие кристаллы, нематические оболочки, гауссова кривизна, топологические дефекты*

Introduction

Study of topological defects (TDs) [1] represents an attractive branch of science both from fundamental and applied perspective. TDs appear unavoidably, at least temporary, in systems with broken continuous symmetry. Consequently, their appearance in nature is ubiquitous, spanning all branches of physics [1, 2]. Due to their topological origin they exhibit several universalities which are independent of microscopic system's details [1, 2].

Particular adequate systems to investigate TDs are various liquid crystalline (LC) phases and structures [3–5]. Namely, LCs are relatively easily experimentally accessible due to their softness (i.e. weak local perturbations could trigger apparent macroscopic-scale responses), optical anisotropy, and rich diversity of different configurations. Because LCs provide a rich environment for precisely controlled experiments they represent an ideal testing ground to study physics of TDs [3–6]. In addition TDs in LCs could be exploited in increasingly broad range of technological and biomedical applications [7, 8].

Nematic phase represents the simplest LC configuration, exhibiting only long range orinetational order [3–8]. In bulk equilibrium anisotropic LC molecules tend to align homogenously along a single symmetry breaking direction. In mesoscopic description nematic ordering is at the simplest level represented by the nematic director field $\vec{n}$ [3–6]. The unit field $\vec{n}$ points along an average local uniaxial ordering, where states $\pm\vec{n}$ are physically equivalent. TDs refers to regions where $\vec{n}$ is not uniquely defined. In LCs there exist either point or line TDs. Their key signature is the topological charge [1, 4] which is a conserved property.

At cores of defects nematic ordering is strongly perturbed and for this reason essentially melted and in general biaxial [4, 8, 9]. Consequently, local LC ordering needs to be described in terms of a nematic tensor order parameter [1, 8, 9].

In the last decade nematic shells [10–13] have become topic of hot interest. A typical LC shell consists of a rigid micrometer-sized colloidal particle coated with a thin sheet of nematic LC subject to degenerate tangential anchoring. Such systems promise various potential applications. For example, they could pave path towards formation of self-assembled scaled crystals, where TDs would play the role of valences [10]. Therefore, TDs would directly influence symmetry of a resulting crystal structure which has strong impact on physical properties. Therefore, it is of strong interest to understand which parameters could sensitively control number and position of TDs in LC shells.

Nematic shells are effectively two-dimensional (2D) and consequently the topological charge of TD is equivalent to its winding number m [4]. The latter is defined as the number of revolutions of $\vec{n}$ divided by 2π on going once around the defect's core. Due to the head-to-tail symmetry of $\vec{n}$, in addition to integers, half integer values of m are also allowed. By the Poincare theorem [14, 15] the topology of a LC shell surface determines the total topological charge m_{tot} within it. For example, $m_{\text{tot}}=2$ for the spherical topology. Vitelli and Nelson [11] were the first to show that spherical shells exhibit four $m = 1/2$ which tend to maximize their mutual separation if anisotropy of elastic constants is not taken into account. Latter studies show that elastic anisotropy, geometry and external fields could have strong impact both on number and position of TDs [12, 13, 16–18]. Furthermore, using simple 2D XY modelling of similar systems reveal analogy with electrostatics [19]. In this analogy m and the Gaussian curvature play the role of the electrical charge and smeared electrical charge respectively.

In this contribution we study impact of curvature on number and position of topological defects in nematic shells exhibiting spherical topology using a mesoscopic tensorial approach. The plan of the paper is as follows. The model used is defined Sec. II. Our numerical results are presented in Sec. III and discussed in the last section.

Model

We model two-dimensional orientational order within a thin LC layer with the nematic tensor order parameter. In the diagonal form we define it as

$$\underline{Q} = \lambda(\vec{n}\otimes\vec{n} - \vec{n}_{\perp}\otimes\vec{n}_{\perp}), \qquad (1)$$

where details are given in [13,16]. Here λ is the positive eigenvalue of $\underline{Q}$ and the unit vectors $(\vec{n}, \vec{n}_{\perp})$ are the eigenvectors corresponding to the eigenvalues $(\lambda, -\lambda)$. We henceforth refer to $\vec{n}$ as the *nematic director field* because it plays a similar role as the conventional uniaxial nematic director field in 3D [1, 4].

We express the corresponding total free energy density potential as [13, 16]

$$f = A_0\left(\frac{T-T_c}{T_c}\right)Tr\underline{\underline{Q}}^2 + \frac{B}{2}\left(Tr\underline{\underline{Q}}^2\right)^2 + k\left|\nabla_s \underline{\underline{Q}}\right|^2, \quad (2)$$

where A_0, B are material constants, T is the absolute temperature, T_c determines the isotropic-nematic phase transition within undistorted flat LC film, k is the nematic elastic constant, and ∇_s stands for the surface gradient [13] and *Tr* stands for the trace operation. The condensation part of f is minimised for

$$\lambda = \lambda_b \equiv \sqrt{\frac{A_0}{2B}\left(\frac{T_c-T}{T_c}\right)}. \quad (3)$$

Note that we use the simplest possible model in order to demonstrate key phenomena of our interest. We work in the approximation of a single nematic elastic constant [13, 16]. Therefore, we do not consider features related with anisotropy of elastic constants.

We focus on nematic ordering within thin closed surfaces, the so called nematic shells [10]. Their surfaces are defined with the position vector

$$\vec{r} = \rho(v)\cos(u)\vec{e}_x + \rho(v)\sin(u)\vec{e}_y + z(v)\vec{e}_z, \quad (4)$$

$$\rho = b\sin(v) + c\sin(3v), \quad (5a)$$

$$z = a\cos(v), \quad (5b)$$

where the Cartesian coordinate system (*x, y, z*) is defined by the unit vector triad ($\vec{e}_x, \vec{e}_y, \vec{e}_z$). The surface of a given geometry is parametrized by parameters (*u, v*), where $u \in [0, 2\pi[$, $v \in [0, \pi[$. Therefore, structures of our study are axially symmetric about the *z*-axis and exhibit the inversion symmetry. Ellipses are obtained for $c = 0$ (where a sphere corresponds to $a = b$). Dumb-bell type geometries are obtained on varying *c*. The Gaussian curvature of a surface is defined by the equation

$$K = \tfrac{1}{2}\left(\left(Tr\left(\nabla_s \vec{v}\right)\right)^2 - Tr\left(\nabla_s \vec{v}\right)^2\right), \text{ i. e.}$$

$$K = -\frac{z_{,v}(z_{,v}\rho_{,vv} - \rho_{,v}z_{,vv})}{\rho(\rho_{,v}^2 + z_{,v}^2)^2}, \quad (6)$$

where $\vec{v}$ stands for the local surface normal, and $A_{,v} = \frac{\partial A}{\partial v}$, $A_{,vv} = \frac{\partial^2 A}{\partial v^2}$. Note that according to the Gauss-Bonnet theorem [13, 15, 16] it holds

$$\frac{1}{2\pi}\oiint K d^2\vec{r} = m_{tot} \quad (7)$$

for surfaces exhibiting in-plane orientational ordering. Here integration is performed over the closed surface and m_{tot} stands for the total topological charge of the *nematic director field*. According to the Poincare theorem [14] it also holds

$$m_{tot} = \chi = 2(1-g), \quad (8)$$

where χ is the Euler-Poincare characteristics of the closed surface and g is its genus (equals to the number of «handles» of the surface). For example, spherical (toroidal) topology is characterized by $g = 0$ ($g = 1$), consequently $m_{\text{tot}} = 2$ ($m_{\text{tot}} = 0$).

For convenience we introduce also the total smeared *Gaussian curvature topological charge* Δm_g within a surface area ΔA as

$$\Delta m_g = -\frac{1}{2\pi}\iint_{\Delta A} K d^2\vec{r}, \quad (9)$$

where the integration is carried over ΔA. If integration is performed over the whole closed surface one obtains $\Delta m_g + m_{tot} = 0$. In case that a surface possesses patches characterised by significantly different average Gaussian curvature, then within each such patch of area ΔA there is a tendency

$$\Delta m_g + \Delta m_{tot} = 0, \quad (10)$$

where Δm_{tot} stands for the total topological charge within ΔA. This equation expresses the tendency that "real" topological charges tend to neutralize local smeared *Gaussian curvature topological charges* [19].

In our simulations we introduce a characteristic linear scale R which measures the width of the central part of axially symmetric structures. An important role is also played by the nematic order parameter correlation length which we define in the nematic phase as

$$\xi = \sqrt{\frac{A_0 T_c}{k(T_c - T)}}, \qquad (11)$$

For a given geometry, defined by dimensionless parameters $\alpha = a / R$, $\beta = b / R$, $\gamma = c / R$, we calculated numerically equilibrium LC structures deep in the nematic phase, where details are given in [13, 16].

Numerical simulations

We numerically investigate impact of curvature on position and number of TDs within thin nematic LC shells exhibiting spherical topology. The latter enforces the total topological charge $m_{tot} = 2$. Simple 2D XY modelling suggests that interactions among TDs and their coupling with the Gaussian curvature bears strong analogy with electrostatics [19]. According to this analogy TDs possessing positive (negative) m are attracted to regions exhibiting maximal positive (minimal negative) value of K. To test validity of these predictions in our more complex description, based on the tensorial order parameter exhibiting quadrupolar symmetry, we continuously vary local curvature of LC films, while preserving the axial rotational symmetry of geometries, and monitor behaviour of TDs. Of particular interest is whether geometries with neighbouring regions exhibiting positive and negative K could trigger unbinding of pairs ($m = 1/2$, $m = -1/2$) of TDs.

In simulations we focus on impact of spatially dependent Gaussian curvature on position and number of TDs. In Fig. 1 we plot some representative spatial profiles of K in structures of our interest. Different patterns of TDs are depicted in Fig. 2. In our simulations we originated from a perfect spherical geometry or radius R. In this case the Gaussian curvature $K = 1/R^2$ is spatially constant and positive. Within our minimal model we obtain four $m = 1/2$ TDs (see the 1st row of Fig. 2) as already predicted by Vitteli and Nelson [11] using simpler model and also studied in detail in [13, 16]. In this case relative positions of TDs are dominated by their mutual repulsion. Consequently, they occupy vertices of a "virtual tetrahedron" touching the spherical surface in order to maximise their mutual separation.

We proceed by continuously squeezing the shell geometry, while preserving the mirror symmetries (see the configurations below the 1st row in Fig. 2), in order to introduce regions with $K<0$ in the neck of resulting structures as shown in Fig. 1. We henceforth refer to the upper and bottom region with $K > 0$ as the *positive Gaussian surfaces* and to the neck area exhibiting $K<0$ as the *negative Gaussian surface.* One sees (Fig. 2, the 2nd row) that four TDs with $m > 0$ tend to move towards regions exhibiting maximal positive K as expected. This is clearly visible by comparing $\lambda(u,v)$ and $\vec{n}(u,v)$ configurations in the 1st and 2nd row.

When a value of $K < 0$ within the neck area reaches the critical value, it triggers local nucleations of two pairs of TDs. Here each pair consists of ($m = 1/2$,$m = -1/2$). A typical configuration is shown in the 3rd row in Fig. 2. Two created TDs bearing $m = 1/2$ ($m = -1/2$) are after their creation pushed towards areas exhibiting maximal positive (maximal negative) value of K in order to partially screen the effective smeared *Gaussian curvature topological charge.*

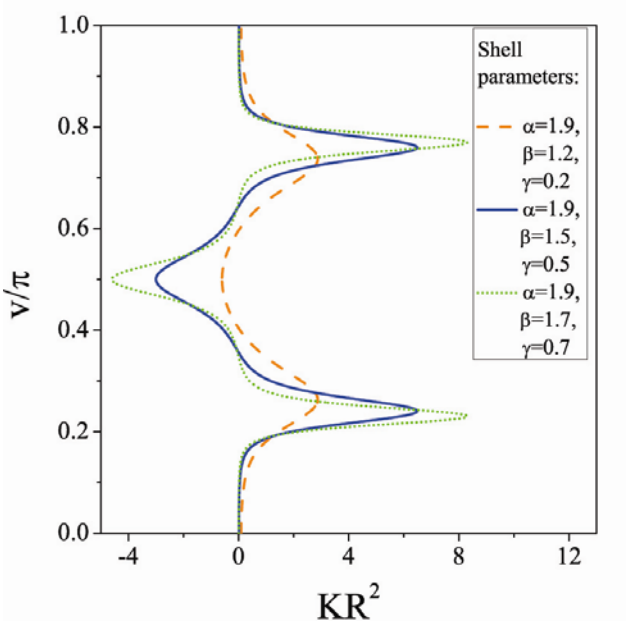

Fig. 1. Spatial variation of the Gaussian curvature. The resulting structures possess surface patches exhibiting $K > 0$ and $K < 0$. $\xi / R = 6$.

On further squeezing the geometry additional two pairs ($m = 1/2$, $m = -1/2$) of TDs appear, see the 4th row in Fig. 2. The resulting equilibrium profile consists now of four $m = 1/2$ TDs within each *positive Gaussian surface* and four $m = -1/2$ TDs within the *negative Gaussian surface*, respectively.

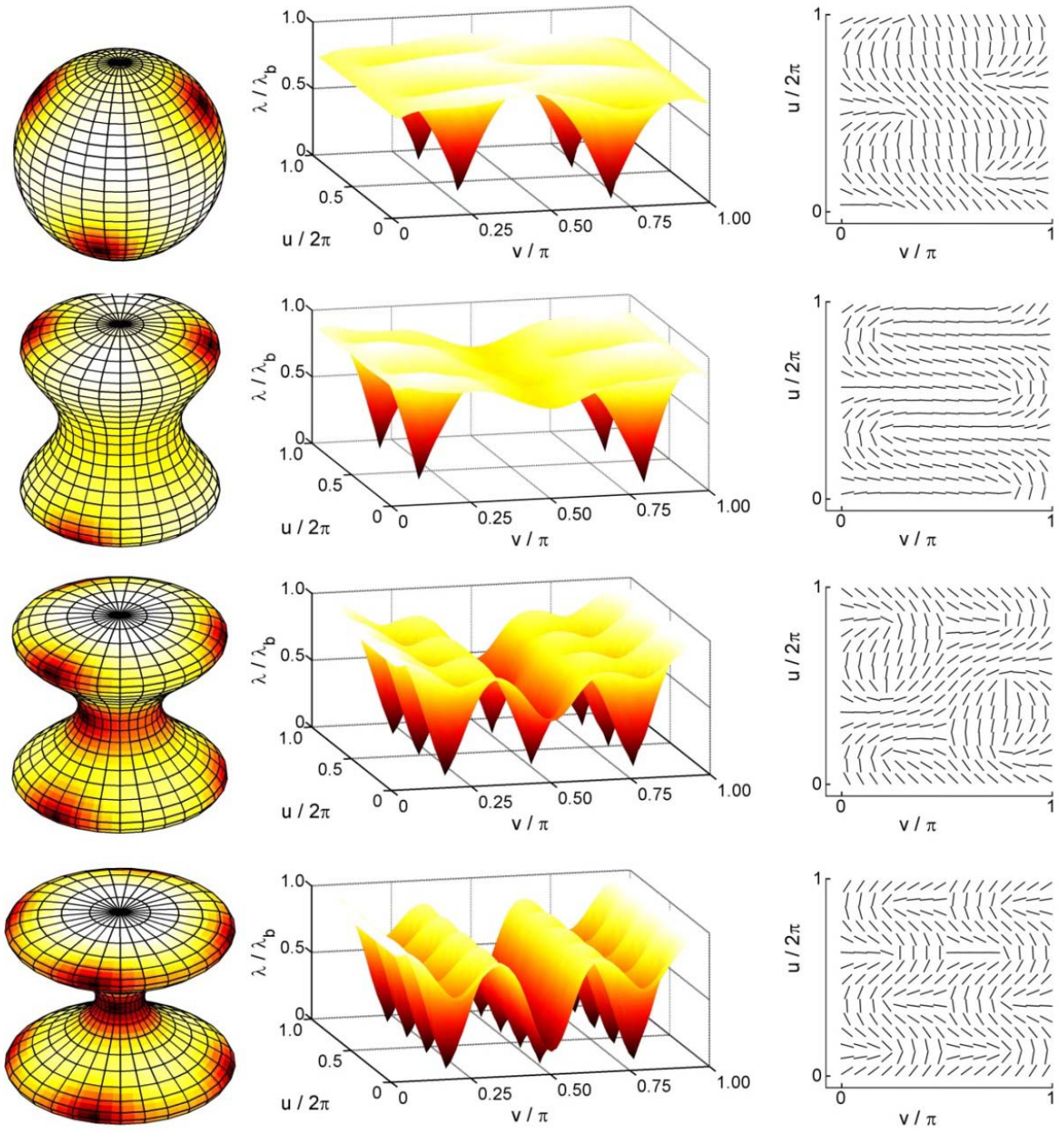

Fig. 2. The nematic order parameter spatial variations within thin LC layers. The left column: Colour plot of λ within LC layers covering different closed geometries exhibiting spherical topology, enforcing m_{tot} = 2. The middle column: Spatial variation of λ in the *(u,v)* plane. The right column: the director field orientation within the (*u,v*) plane. The 1st ($\alpha = \beta = 1,\ \gamma = 0$) and 2nd row ($\alpha = 1.9,\ \beta = 1.2,\ \gamma = 0.2$): four TDs with *m*=1/2. The 3rd row ($\alpha = 1.9,\ \beta = 1.2,\ \gamma = 0.5$): eight TDs, six TDs with *m* = 1/2 and two with *m* = -1/2. The 4th row ($\alpha = 1.9,\ \beta = 1.2,\ \gamma = 0.7$): twelve TDs, eight TDs with *m* = 1/2 and four with *m* = -1/2. The corresponding plots of *K* as shown in Fig. 1. $R / \xi = 6$.

Note that further squeezing the structures do not any more qualitatively change configurations of TDs. Namely integration over each *positive Gaussian surface* yields $\Delta m_g = -2$. On the other hand the integration over the *negative Gaussian surface* yields $\Delta m_g = 2$. Therefore, the total compensation of these smeared *Gaussian topological charges* within each *positive (negative) Gaussian surface* requires presence of four $m = 1/2$ ($m = -1/2$) TDs, respectively, in order to fulfil Eq. (1).

Conclusions

We studied impact of the Gaussian curvature in effectively 2D LC surfaces exhibiting in-plane orientational order. We consider axially symmetric closed structures, also referred to as nematic shells. In particular we focus on dumb-bell shells possessing spherical topology. In this case the total topological charge within a shell equals $m_{\text{tot}} = 2$.

We use a Landau-type minimal model where the degree of local orientational ordering is described in terms of the tensor order parameter. Equilibrium profiles were calculated by numerical minimization of the free energy functional. Due to the approximation of equal nematic elastic constants we obtain within a spherical shell four TDs bearing $m = 1/2$ residing in vertices of a hypothetical tetrahedron in line with previous studies [11]. Such configuration of TDs maximizes their mutual separation. On gradually squeezing initial spherical geometry we obtain dumb-bell geometries, possessing regions exhibiting both positive and negative local Gaussian curvatures. One sees that in initial stages the four $m = 1/2$ tend to be pushed towards regions exhibiting maximal Gaussian curvature as the electrostatic analogy suggests [19]. According to it "real" discrete topological charges tend to neutralise the locally smeared *Gaussian topological charge* concentrated within regions displaying maximal values of K. On further squeezing the geometry the Gaussian curvature at the neck of dumb-bell becomes negative enough to trigger unbinding of two pairs ($m = 1/2$, $m = -1/2$) of TDs in order to more efficiently compensate Δm_g. Finally, in relatively strongly distorted dumb-bell structure we obtain completely compensated *Gaussian topological charges* in all areas of a dumb-bell structure.

Results of our simulations are of interest also for research dealing with biological membranes [20–23]. Namely, as first pointed out in [20] the coupling between in-plane ordering within a membrane and its curvature might have strong impact on the membrane shape. In particular presence of TDs in ordering gives rise to presence of spatial inhomogeneities which might enable local membrane processes important for biological cell viability.

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