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Impact of curvature on topological defects

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Abstract. We analyze the impact of *extrinsic* and *intrinsic* curvature on positions of topological defects (TDs) in two-dimensional (2D) nematic films. We demonstrate that both these curvature contributions are commonly present and are expected to be weighted by comparable elastic constants. A simple Landau-de Gennes approach in terms of tensor nematic order parameter is used to numerically demonstrate impact of the curvatures on position of TDs on 2D ellipsoidal nematic shells. In particular, in oblate ellipsoids the *extrinsic* and *intrinsic* elastic terms enforce conflicting tendencies to positions of TDs.

1. Introduction

Topological defects [1] (TDs) represent a popular interdisciplinary subfield of science. For years, they are of hot interest in particle physics, condensed matter physics and even cosmology [2,3]. The reason for their popularity in all fields of science is their topological origin [1], which is blind for systems' microscopic details. In particular, there is growing evidence that *fields* represent basic entities of nature [4], and not “fundamental particles” as pictured by the Standard Model of nature. If this is the correct view than “fundamental particles” are emergent and correspond to relatively stable localized structures in a relevant *field*. Possible candidates for them are TDs as pioneering work of Skyrme suggests [5]. He has shown that pions, nuclear particles belonging to the meson family, could be represented as TDs in a relevant *field*. In the following years, mathematically related TDs, which are referred to as Skyrmions, have been detected and studied in more details in numerous different condensed matter systems [6,7,8] (e.g. in magnetism, liquid crystals...). Namely, due to interdisciplinary nature of TDs it is convenient to find experimentally adequate systems where static and dynamic fundamental properties of TDs could be relatively easily accessed [2].

The key property of TDs is their discrete topological charge q [2,3]. In general, topological charges play analogous role to electric charges: i.e., q of an isolated TD is conserved and a pair of TDs bearing opposite charge attract each other. Pairs of TDs bearing $\{q>0, -q\}$ are referred to as $\{\text{defect}, \text{antidefect}\}$ and have tendency to annihilate into a defect-less state. By contrast, TDs bearing the same sign of



topological charges in general repel. In two-dimensions (2D) the topological charge is equivalent to the so called winding number m [3]. It quantifies the total rotation of the relevant orientational field divided by 2π on encircling the core of defect counterclockwise.

An adequate experimental testing bed to study TDs are liquid crystal (LC) phases [9]. In general, LC phases could be formed if they consist of relatively weakly interacting anisotropic molecules. For simplicity we henceforth restrict to thermotropic rod-like LC molecules, where LC ordering is stabilized in an adequate temperature interval. LC owe their experimental accessibility to unique combination of fluidity, softness, and optic anisotropy. Due to rich diversity of their configurations they can possess any topological defect configuration [2]. For instance, their structure could be relatively easily studied using optic polarizing microscopy. Nematic configurations represent simplest LC structures. In the nematic bulk phase LC molecules tend to be homogeneously aligned along a single symmetry breaking axis, while centers of masses of molecules flow roughly like in a fluid.

Effectively two-dimensional nematic LC structures are of particular interest. First of all, they are relatively easily accessible for mathematical and numerical investigations. Secondly, such structures are of interest for various applications, in particular those exhibiting TDs. For instance, nematic shells [10,11] consisting of supra micron-sized colloids covered with relatively thin LC films are of interest for various photonic applications. Furthermore, biological membranes are essentially thin LC films [12,13]. So far, in almost all theoretical attempts, covariant derivatives [13,14,15] were employed in expressing free energy elastic terms of 2D ordered systems. Such approaches took into account only the so called *intrinsic* curvature [16] elasticity which is associated with spatial variations of a relevant orientational field within the curved surface. It has been shown that in this case surface regions with high absolute value of the Gaussian curvature attract TDs [14,15,17,18]. Furthermore, electrostatic analogy works well where positive (negative) Gaussian curvature plays similar role as spread negative (positive) topological charge of TDs [14,18]. However, recently it has been demonstrated that *extrinsic* curvature [16,19,20] elasticity terms are in general also present and could have important impact on resulting structures. This elasticity takes into account that a curved 2D manifold is embedded in 3D geometry. In some cases a structure could simultaneously maximize and minimize *intrinsic* and *extrinsic* free energy costs contributions and vice versa [16,19].

In the present paper we demonstrate relative importance of *intrinsic* and *extrinsic* terms on orientational ordering within nematic shells exhibiting spherical topology. For simplicity we restrict to structures displaying cylindrical symmetry. We first demonstrate using a minimal model that both contributions are in general present. Then we numerically demonstrate cases, where *extrinsic* elasticity could play significant role.

2. *Intrinsic* and *extrinsic* curvature

We consider a thin nematic LC film and describe local orientation of LC molecules by the unit vector field $\vec{n}$ lying within a curved 2D film. We consider rod-like LC molecules, therefore the orientations $\pm\vec{n}$ are equivalent. For illustration purpose we chose the simplest possible free energy density expression $f = k|\nabla_s \vec{n}|^2$ [9]. Here k is the positive elastic constant, the operator $\nabla_s = (\underline{I} - \vec{v} \otimes \vec{v})\nabla$ is the surface gradient [17], $\underline{I}$ is the 3D identity tensor, ∇ is the conventional 3D gradient operator, $\vec{v}$ is the surface normal, and $\otimes$ is the tensorial product.

It is convenient to parametrize $\vec{n}$ in the surface principal curvature frame $(\vec{e}_1, \vec{e}_2)$ in which the curvature tensor $\underline{C} = C_1 \vec{e}_1 \otimes \vec{e}_1 + C_2 \vec{e}_2 \otimes \vec{e}_2$ is diagonal, $\{C_1, C_2\}$ are the corresponding principal curvatures, and $\vec{v} = \vec{e}_1 \times \vec{e}_2$. Therefore

$$\vec{n} = \vec{e}_1 \cos\vartheta + \vec{e}_2 \sin\vartheta. \quad (1)$$

Taking into account equations [21]

$$\nabla_s \vec{n} = \cos\vartheta \nabla_s \vec{e}_1 - \sin\vartheta \vec{e}_1 \otimes \nabla_s \vartheta + \sin\vartheta \nabla_s \vec{e}_2 + \cos\vartheta \vec{e}_2 \otimes \nabla_s \vartheta, \quad (2a)$$

$$\nabla_s \vec{e}_1 = \kappa_{g1} \vec{e}_2 \otimes \vec{e}_1 + \kappa_{g2} \vec{e}_2 \otimes \vec{e}_2 - C_1 \vec{v} \otimes \vec{e}_1, \quad (2b)$$

$$\nabla_s \vec{e}_2 = -\kappa_{g1} \vec{e}_1 \otimes \vec{e}_1 - \kappa_{g2} \vec{e}_1 \otimes \vec{e}_2 - C_2 \vec{v} \otimes \vec{e}_2, \quad (2c)$$

it follows

$$|\nabla_s \vec{n}|^2 = |\nabla_s \vartheta + \vec{A}|^2 + \vec{n} \cdot \underline{C}^2 \vec{n}, \quad (3a)$$

$$\vec{A} = \kappa_{g1} \vec{e}_1 + \kappa_{g2} \vec{e}_2. \quad (3b)$$

Here $\{\kappa_{g1}, \kappa_{g2}\}$ are geodesic curvatures along $\{\vec{e}_1, \vec{e}_2\}$, $\vec{A}$ is the spin connection [22], which can be expressed in terms of the Gaussian curvature $K = C_1 C_2$ as $K = |\nabla \times \vec{A}|$.

Therefore, the free energy density could be expressed as the sum $f = f^{(int)} + f^{(ext)}$ of *intrinsic* ($f^{(int)}$) and *extrinsic* ($f^{(ext)}$) elastic contributions, where

$$f^{(int)} = k |\nabla_s \vartheta + \vec{A}|^2, \quad (4a)$$

$$f^{(ext)} = k \vec{n} \cdot \underline{C}^2 \vec{n} = k (C_1 \cos^2 \vartheta + C_2 \sin^2 \vartheta). \quad (4b)$$

The *intrinsic* term enforces homogeneous orientational ordering for surfaces characterized by $K=0$. By contrast, surface patches with nonzero Gaussian curvature are geometrically frustrated. Consequently, spatially nonhomogenous ordering minimizes $f^{(int)}$. More exactly, a local orientational structure obeys the so called parallel transport condition [21]:

$$\nabla_s \vec{n} = -(\vec{v} \otimes \underline{C}) \vec{n}. \quad (5)$$

It originates from the incompatibility of straight-parallel direction on surfaces with $|K| > 0$. Using the parametrization Eq.(1) the condition yields $\nabla_s \vartheta = -\vec{A} = -(\kappa_{g1} \vec{e}_1 + \kappa_{g2} \vec{e}_2)$, and consequently $f^{(int)} = 0$. Note that the approaches employing covariant derivatives yield only the *intrinsic* contribution.

The *extrinsic* term acts as an effective external field. Namely, it tends to align $\vec{n}$ along the principal direction exhibiting minimal curvature.

3. Numerical simulation

In order to demonstrate impact of *extrinsic* curvature we employ a simple Landau-de Gennes type model, where nematic orientational order is represented by the tensor order parameter $\underline{Q}$ [17,21].

3.1. Model

In the diagonal form it can be expressed as

$$\underline{Q} = \eta (\vec{n} \otimes \vec{n} - \vec{n}_\perp \otimes \vec{n}_\perp). \quad (6)$$

Here $\eta \in [0, 1/2]$ and $-\eta$ are eigenvalues of eigenvectors $\vec{n}$ and $\vec{n}_\perp$, respectively. Localised points on 2D manifolds exhibiting nematic ordering in general reveal presence of TDs. We calculate the degree of nematic ordering by minimizing the relevant free energy of a system. We express the relevant dimensionless free energy density as [17,19,20]

$$f = \left(\frac{R}{\xi_0}\right)^2 \left(t \left| \underline{Q}^2 \right| + \left| \underline{Q}^2 \right|^2 + k_i \left| \nabla_s \underline{Q} \right|^2 + k_e \underline{Q}^2 \cdot \underline{C} \right). \quad (7)$$

Here R is a geometrically imposed length characterizing a system, ξ_0 estimates the order parameter length deep in the nematic phase, the quantity $t = (T - T_c)/T_c$ is the reduced temperature, T_c is the critical temperature below which spatially homogeneous nematic ordering is stable on a flat surface. The relative strength of $\{intrinsic, extrinsic\}$ elastic contribution is weighted by dimensionless constants $\{k_i, k_e\}$, where we set $k_i = 1$.

In simulations we consider ellipsoidal shapes which we parametrize in the Cartesian system (x, y, z) determined by the unit vectors $(\vec{e}_x, \vec{e}_y, \vec{e}_z)$ as

$$\vec{r} = b(\sin(v) \cos(u) \vec{e}_x + \sin(v) \sin(u) \vec{e}_y) + a \cos(v) \vec{e}_z. \quad (8)$$

The position vector $\vec{r}$ determines a point on an ellipsoidal surface, $v \in [0, \pi]$, $u \in [0, 2\pi]$, and R in Eq.(7) corresponds to the minimal length of the pair $\{a, b\}$. The ellipsoidal shells are prolate for $a/b > 1$ and oblate for $a/b < 1$. More details are given in [17].

3.2. Nematic textures

In figures 1 we plot a typical nematic structure on a spherical shell ($a/b=1$). In figure 1a we plot superimposed scalar order parameter η and the orientational field $\vec{n}$, where states $\pm \vec{n}$ are equivalent. The corresponding scalar order parameter graph in the (u, v) plane, which clearly reveals position of four TDs bearing topological charge $m=1/2$, is shown in figure 1b. The quantity η_c determines the equilibrium value of η in a flat film. In this case the *extrinsic* term is absent because both principal curvatures are equal. The TDs are placed in such a way to maximize their mutual separation, because TDs repel each other.

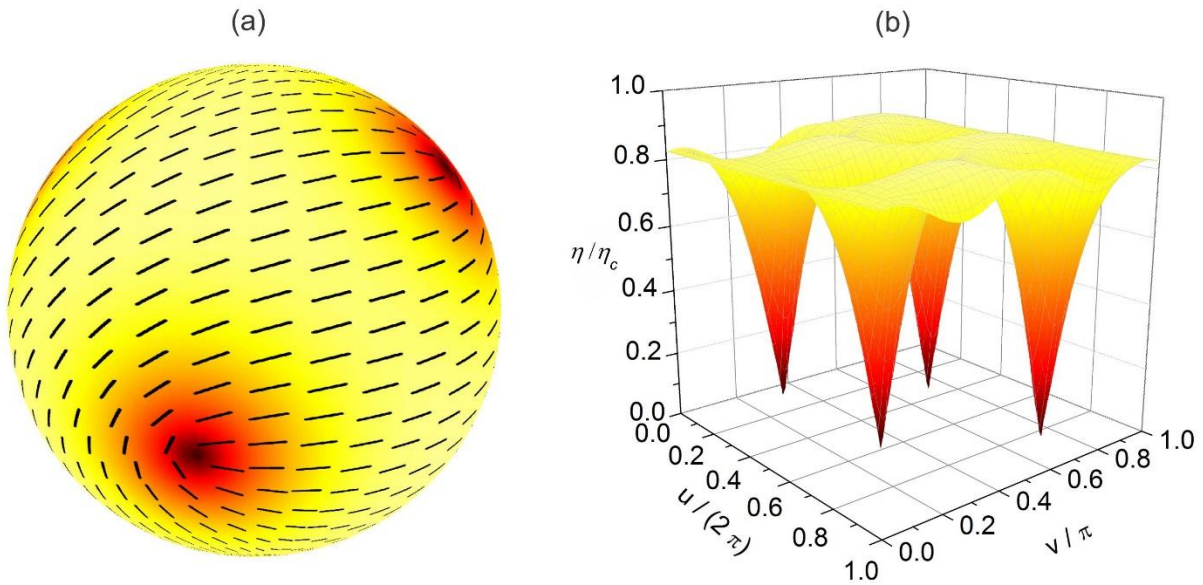


Figure 1. Typical nematic ordering on a spherical shell. The color code represents the η/η_c ratio. The panel (a) also shows the directions of molecules on a sphere. The panel (b) represents the calculated nematic texture in the (u, v) -plane. Parameters: $a/b = 1$, $R/\xi_0 = 20$, $k_i = 1$, $k_e = 0$, $t = -0.03$.

Next we deform spheres to form oblate and prolate ellipsoids. In figures 2 (nematic textures depicted on ellipsoidal shapes) and figures 3 (nematic textures in the (u, v) plane) we demonstrate impact of shape and extrinsic curvature on position of TDs. We first consider cases for $k_e = 0$ for which

the *extrinsic* elasticity is absent. A typical nematic texture for a prolate structure for is shown in figure 2a and figure 3a. TDs are pushed towards the poles because they are attracted by the positive Gaussian curvature, which exhibits maximum at the poles, see figure 4a. This attraction of TDs bearing positive topological charges with regions exhibiting $K > 0$ competes with the mutual repulsion among TDs. Note that for strong enough prolateness pairs of $m=1/2$ TDs merge into $m=1$ TDs localized at poles of ellipsoids [17]. In oblate structures K exhibits maximum at the equatorial great circle as figure 4a demonstrates. In figure 2b and figure 3b we show a case where attraction between $K > 0$ and TDs is strong enough to localize TDs at the equatorial circle.

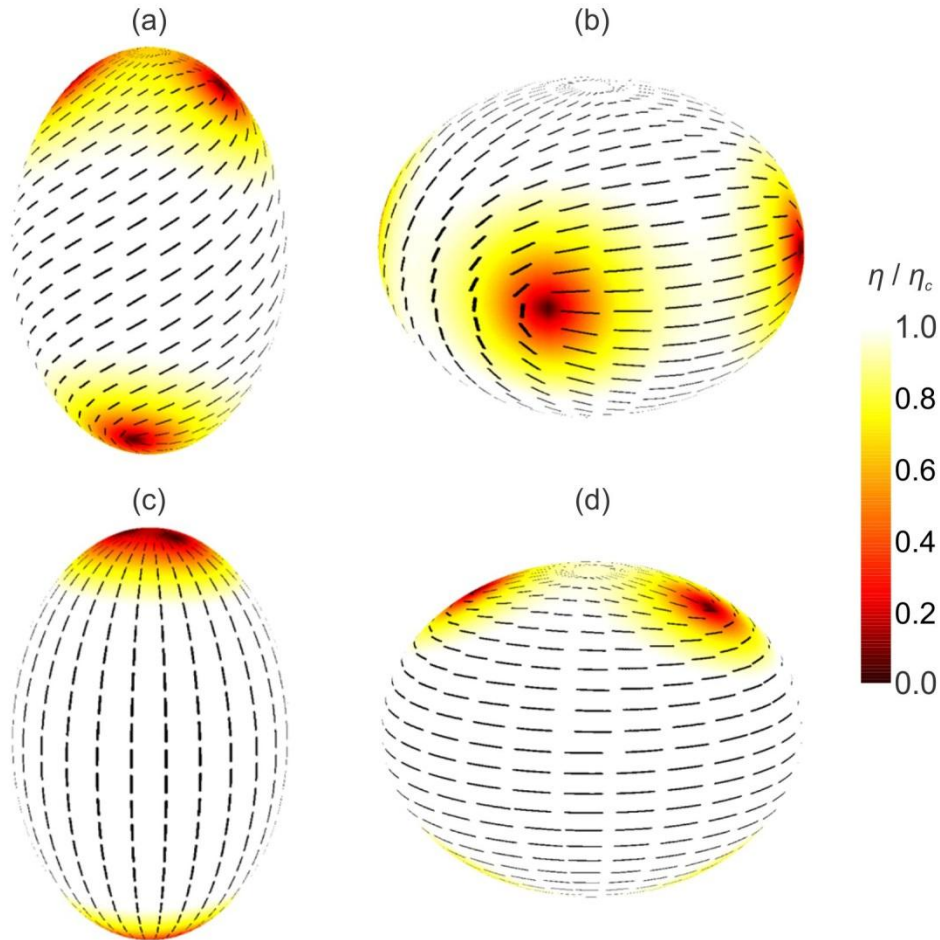


Figure 2. The degree of nematic ordering and the directions of molecules on prolate $a/b = 1.5$ (a,c) and oblate $b/a = 1.28$ (b,d) ellipsoids. The nematic textures in panels (c) and (d) show the impact of the *extrinsic* elastic contribution: $k_e = 1$, while the configurations in panels (a) and (b) were calculated without the extrinsic term: $k_e = 0$. Other parameters were set as follows: $R/\xi_0 = 20$, $t = -0.03$.

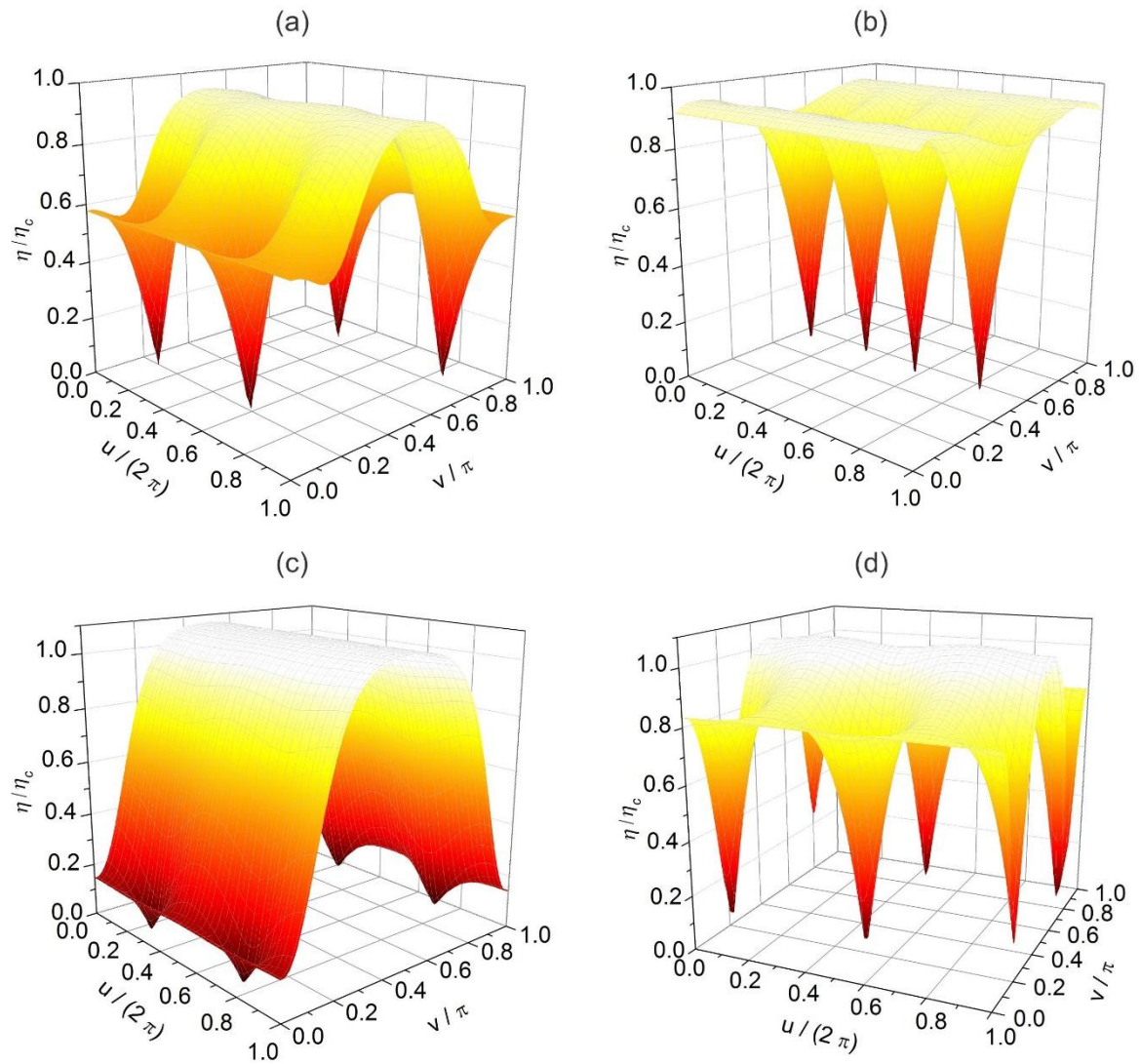


Figure 3. Representation in the (u, v) -plane of the nematic textures presented in figure 2. Parameters are defined in the figure caption of figure 2.

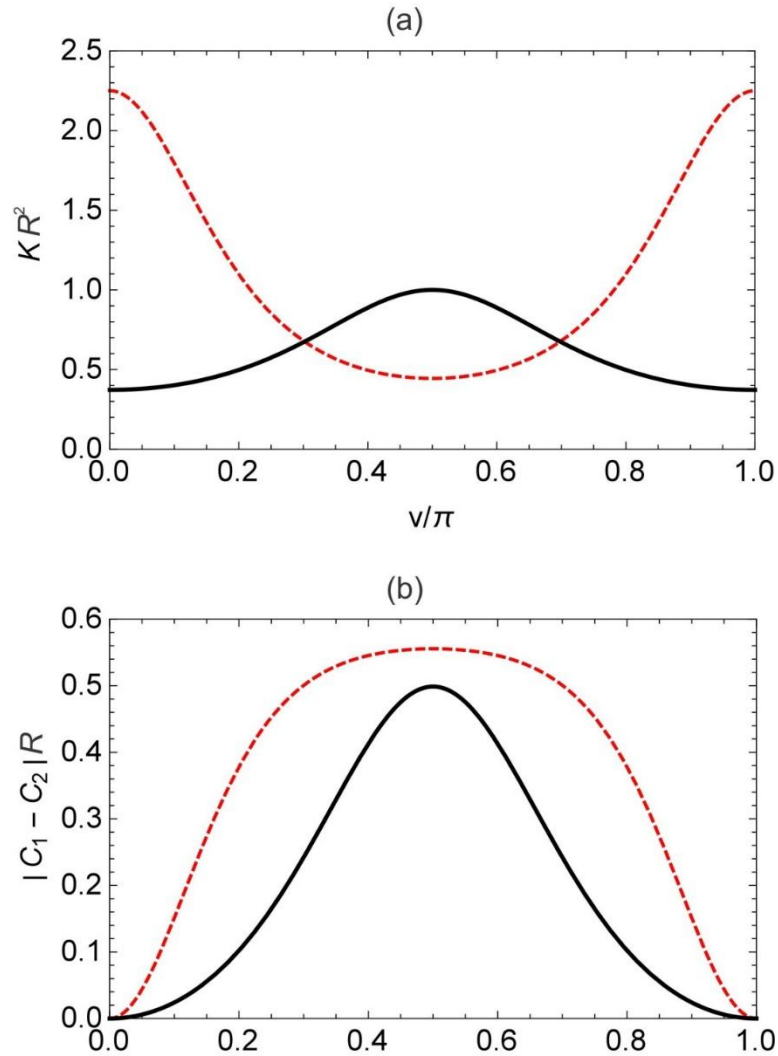


Figure 4. Gaussian curvature K (a) and the absolute difference between the principal curvatures $|C_1 - C_2|$ (b) as the functions of the ellipsoid's zenith angle v . Red dashed lines represent the prolate ellipsoid $a/b = 1.5$, while the black lines represent the oblate ellipsoid $b/a = 1.28$.

In prolate and oblate structures in general principal curvatures differ, i.e. $C_1 \neq C_2$. Consequently, for a finite value of k_e the *extrinsic* elasticity could play important role. For $k_e > 0$ it tends to align nematic orientational ordering along principal directions exhibiting minimal curvature. This tendency is monotonously increasing with increasing difference $|C_1 - C_2|$, which is shown in figure 4b. Note that the resulting effective *extrinsic* field tends to align nematic ordering along its direction. Therefore, TDs tend to be expelled from regions where the effective *extrinsic* field is strong enough. In both prolate and oblate structures the difference $|C_1 - C_2|$ exhibits maximum in equatorial region. Consequently, in prolate structure TDs are pushed by the effective *extrinsic* field towards the poles, see figure 2c and figure 3c. In this case both *intrinsic* and *extrinsic* term are pushing TDs towards the poles. By contrast, in oblate structure the *intrinsic* and *extrinsic* term have competing tendencies. The *intrinsic* elasticity tends to assemble TDs in the equatorial region, while the *extrinsic* term expels them. In figures 2d and figure 3d we demonstrate cases where the effective *extrinsic* term is strong enough to expel TDs from the equatorial region.

4. Conclusions

We studied impact of curvature on position of topological defects in two-dimensional nematic films. For this purpose we employ Landau-de Gennes type description in terms of nematic tensor order parameter. In particular, we consider the role of *extrinsic* curvature [16,19,20], which has been so far in most studies neglected, see e.g. [13,14,15]. In the latter approaches covariant derivatives of order parameter were employed in expressing elastic free energy compatible with symmetry of systems of interest. Equivalently, it was assumed that minimal elastic distortion in a relevant order parameter field along a given direction obeyed parallel transport concept [21]. In a parallel transport along a line the order parameter experiences the least motion capable accompanying the spatial variation of surface normal. In the setting of our model $\vec{n}$ is parallel transported along a curve if it is seen as immobile in the frame $(\vec{e}_1, \vec{e}_2, \vec{v})$. In such cases it is known that the *intrinsic* curvature of a surface frustrates the order parameter field within the curved 2D space [13,14,15]. For example, for spherical topology the total integrated Gaussian curvature makes defects necessary even in the ground state. Furthermore, *intrinsic* curvature favours localization of TDs in regions of relatively high absolute value of Gaussian curvature.

We showed using a simplest possible modelling that in general both *intrinsic* and *extrinsic* curvature are expected to be present in elastic free energy density. Furthermore, there are no general reasons to claim that *extrinsic* curvature terms should be negligible with respect to the *intrinsic* contributions. The *extrinsic* term quantifies elastic costs of out-of-plane gradients in $\vec{n}$. Therefore, it is sensitive how 2D curved surface is embedded in 3D Euclidian space. The *extrinsic* coupling generates an unavoidable geometrically induced symmetry breaking field on surfaces patches possessing different principal curvatures. Its strength increases with increasing difference between the curvatures and equals zero in umbilic points, where the principal curvatures are equal. To illustrate this effect we calculated nematic structures on ellipsoidal shells. In the spherical geometry the *extrinsic* contribution is absent because all points are umbilics. However, on increasing prolateness or oblateness of shells regions where *extrinsic* curvature is present emerge. In our cases the effective *extrinsic* curvature is strongest at the equator of ellipsoids. Its ordering tendency is incompatible with TDs and it tends to expel them. This effect is most evident in oblate ellipsoids. Namely, the *intrinsic* curvature tends to localize TDs bearing positive topological charge in the equatorial region in order to screen strongly localised Gaussian curvature. However, for equally weighted *intrinsic* and *extrinsic* free energy contributions for strong enough oblateness the TDs are expelled from the equatorial region.

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