Director configurations of a nematic liquid crystal confined in a toroidal geometry. A finite element study.

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Abstract

Various director configurations of a nematic liquid crystal, confined in a toroidal volume and subject to an external magnetic field, were evaluated numerically by performing finite element calculations in three dimensions. The equilibrium director field is found from a minimization of the elasto-magnetic energy of the nematic. The director at the inner surface of the torus is fixed, either along homeotropic or tangential direction. We consider both a homogeneous and an azimuthal magnetic field, with its direction being in conflict with the respective surface anchoring.

The relative stability of topologically inequivalent configurations is investigated in dependence on the strength of the magnetic field and the geometrical parameters of the confining torus. We find that in a toroidal geometry the director “escape” from a disclination, which usually occurs in a cylindrical tube, is absolutely stable only for weak magnetic fields and tangential anchoring, whereas for homeotropic anchoring director fields containing disclination rings are more favorable. When a strong homogeneous magnetic field is exerted laterally, the resulting director field is not any more axially symmetric, instead, it reveals curved disclinations of finite length.

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I. INTRODUCTION

Since the discovery of polymer-dispersed liquid crystals (PDLC) [1, 2, 3] the confinement of nematics in curved geometries attracts considerable interest [4]. Small nematic droplets embedded in a polymer matrix give rise to light scattering effects [5, 6, 7] which are controllable by an external electric field and thus can be applied in electro-optical light shutters of high contrast. On the other hand, from the viewpoint of basic research, nematics confined by curved surfaces are challenging as they exhibit non-trivial director fields. Due to the large surface-to-volume ratio the boundary conditions at the surface strongly influence the emerging structures which reveal a large variety of topological defects [4]. The structure of nematics confined in a spherical droplet or a cylindrical capillary tube has been studied in detail. For the spherical droplet, homeotropic surface anchoring mainly leads to a radial point defect in the center of the droplet [8, 9, 10, 11] or, alternatively, to a defect ring in the equatorial plane of the droplet [12, 13, 14, 15, 16, 17]. Tangential anchoring creates two surface point defects, denoted boojums, at opposite poles of the droplet surface [18, 19]. (For some years, the inverse problem of a nematic surrounding an isotropic spherical droplet has been addressed, too [14, 20, 21, 22, 23, 24].) On the other hand, in a cylindrical geometry, homeotropic or tangential surface anchoring does not lead to a line defect, instead, this disclination generally turns out to be unstable against an “escape” of the director field lines along the symmetry axis of the tube [8, 10, 25, 26, 27].

In our contribution, we consider an advanced scenario, namely, the confinement of a nematic liquid crystal in a torus. This is an elementary paradigm for a nematic filling a volume which is not simply connected. For some years now, the method of finite elements has been applied to the study of liquid crystals and polymers in complex geometries [28, 29, 30]. Accordingly, we performed finite element calculations in three dimensions for a toroidal geometry, thus enabling the investigation of fairly complicated situations. Both homeotropic and tangential boundary conditions for the director field at the torus surface are taken into account. In addition, an external magnetic field is exerted on the nematic whose direction is in conflict with the boundary conditions imposed. By minimizing the elasto-magnetic free energy of the nematic the equilibrium director configurations are found. We discuss the relative stability of various topological defect structures in dependence of the strength of the magnetic field and the geometrical parameters of the confining torus.
The organization of the article is as follows. In Section II the finite element method for director fields in a torus is introduced. Section III presents a survey of equilibrium director configurations for various situations. Finally, Section IV contains some concluding remarks.

II. TOROIDAL GEOMETRY AND FINITE ELEMENT METHOD

The geometry of our system is confined by a torus with its symmetry axis along the \( z \) direction and its large circle in the \( x-y \) plane. The radii of the large and small circle are \( A \) and \( B \), respectively (Figure 1). The torus is filled by a nematic liquid crystal whose director field is fixed at the inner surface of the torus. According to the toroidal geometry there are three distinct boundary conditions of Dirichlet type. Their respective directors at the surface on sections of the torus across the \( x-z \) and \( y-z \) coordinate planes are visualized from an oblique view in Figure 2. (Note that for sake of clarity not all directors that were calculated on the grid are displayed.) The director can be anchored either perpendicular (homeotropic) or tangential to the surface. Tangential anchoring can be established along sections across the small circle of the torus (transversal-tangential) or, alternatively, following the direction of its large circle (azimuthal-tangential). In addition to the boundary conditions at the surface, the director field is affected by an external magnetic field. We examine the influence of both a homogeneous magnetic field and an inhomogeneous magnetic field of axial symmetry. The latter is created by an electric current through a wire of infinite length along the symmetry axis of the torus, giving rise to closed magnetic field lines along the azimuthal direction. Whereas the azimuthal magnetic field as well as the homogeneous field along the \( z \) direction still preserve axial symmetry, this rotational symmetry does not hold any more for a “lateral” homogeneous field along the \( x \) axis. Obviously, for such a scenario, a finite element calculation in three dimensions is necessary.

The particular combinations of boundary conditions and magnetic fields that we considered in our calculations will be introduced in the following section. For each combination the equilibrium director fields are found from a numerical minimization of the free energy \( F \) of the nematic, with the corresponding energy density

\[
\mathcal{F} = \frac{1}{2} K_{11} (\text{div} \mathbf{n})^2 + \frac{1}{2} K_{22} (\mathbf{n} \cdot \text{curl} \mathbf{n})^2 + \frac{1}{2} K_{33} (\mathbf{n} \times \text{curl} \mathbf{n})^2 - \frac{1}{2} \mu_0 \Delta \mu (\mathbf{n} \cdot \mathbf{H})^2. \tag{1}
\]

The first three terms in (1) form the elastic free energy density due to splay, twist and bend...
deformations, respectively, of the director field \( \mathbf{n} \), according to Oseen, Z"ocher and Frank [31]. \( K_{11}, K_{22} \) and \( K_{33} \) are the elastic constants for the three deformation modes mentioned above. The last expression in (1) represents the coupling of the director field to an external magnetic field \( \mathbf{H} \). Here the anisotropy of the magnetic permeability \( \Delta \mu \) of the nematic acts as the coupling strength. (\( \mu_0 \) is the magnetic field constant.)

For numerical treatment, the nematic free energy density (1) is expressed in a dimensionless form, \( i.e., \) in units of \( K_{33}/a^2 \), where \( a \) is a measure for the characteristic length scale of our system (usually in the range of a micron). The director field is determined by the tilt and twist angle, \( \Theta \) and \( \Phi \), respectively,

\[
\mathbf{n} = \hat{x} \sin \Theta \cos \Phi + \hat{y} \sin \Theta \sin \Phi + \hat{z} \cos \Theta.
\]

Therefore, the reduced free energy \( \overline{F} \), \( i.e., \) the volume integral of the free energy density becomes a functional of the tilt and twist angle,

\[
\overline{F}[\Theta, \Phi] = \int d^3x \left\{ \frac{1}{2} \overline{K}_{11} \left[ (\partial_x \Theta \cos \Phi + \partial_y \Theta \sin \Phi) \cos \Theta - \partial_z \Theta \sin \Theta \right] - (\partial_x \Phi \sin \Phi - \partial_y \Phi \cos \Phi) \sin \Theta \right]^2
\]

\[
+ \frac{1}{2} \overline{K}_{22} \left[ \partial_x \Theta \sin \Phi - \partial_y \Theta \cos \Phi + (\partial_x \Phi \cos \Phi + \partial_y \Phi \sin \Phi) \sin \Theta \cos \Theta - \partial_z \Phi \sin^2 \Theta \right]^2
\]

\[
+ \frac{1}{2} \left[ (\partial_x \Theta \cos \Phi + \partial_y \Theta \sin \Phi) \cos \Phi \sin \Theta \cos \Theta + \partial_z \Theta \cos^2 \Theta \cos \Phi \right.
\]

\[
- (\partial_x \Phi \cos \Phi + \partial_y \Phi \sin \Phi) \sin \Phi \sin^2 \Theta - \partial_z \Phi \sin \Theta \cos \Theta \sin \Phi \right]^2
\]

\[
+ \left[ (\partial_x \Theta \cos \Phi + \partial_y \Theta \sin \Phi) \sin \Phi \sin \Theta \cos \Theta + \partial_z \Theta \cos^2 \Theta \sin \Phi \right.
\]

\[
+ (\partial_x \Phi \cos \Phi + \partial_y \Phi \sin \Phi) \cos \Phi \sin^2 \Theta + \partial_z \Phi \sin \Theta \cos \Theta \cos \Phi \right]^2
\]

\[
+ \left[ (\partial_x \Theta \cos \Phi + \partial_y \Theta \sin \Phi) \sin^2 \Theta + \partial_z \Theta \sin \Theta \cos \Theta \right]^2 \right) - \frac{1}{2\xi} \left[ h_x \sin \Theta \cos \Phi + h_y \sin \Theta \sin \Phi + h_z \cos \Theta \right]^2 \right\}.
\]

In (3), all lengths are in reduced units of \( a \). The reduced elastic constants are \( \overline{K}_{11} = K_{11}/K_{33} \) and \( \overline{K}_{22} = K_{22}/K_{33} \). \( \overline{\xi} = \xi/a \) is the reduced magnetic coherence length, with \( \xi = \sqrt{K_{33}/(\mu_0 \Delta \mu)} \cdot (1/H) \). \( H \) is the strength of the magnetic field \( \mathbf{H} \) and \( (h_x, h_y, h_z) \) are the Cartesian components of the local unit vector along the direction of \( \mathbf{H} \). For the homogeneous magnetic field this unit vector is constant along the \( z \) or \( x \) direction, whereas for the azimuthal field it becomes \((-y/\rho, x/\rho, 0)\), with cylindrical coordinate \( \rho = \sqrt{x^2 + y^2} \).
The parametrization of our calculations is based on the nematic liquid crystal pentyl-cyanobiphenyl (5CB) [32]. Its elastic constants are $K_{11} = 4.2 \times 10^{-12} \text{ N}$, $K_{22} = 2.3 \times 10^{-12} \text{ N}$, $K_{33} = 5.3 \times 10^{-12} \text{ N}$, which amounts in the ratios $\overline{K}_{11} = 0.79$ and $\overline{K}_{22} = 0.43$. The strength of the magnetic field is varied from zero up to $1.5 \times 10^7 \text{ A/m}$ which, with a magnetic anisotropy of $1.2 \times 10^{-7}$, means a reduced inverse coherence length in the range between zero and 2.5. Besides the magnetic coherence length, the geometrical parameters of the confining torus are changed. Its large radius ranges from $A = 7$ to 9, whereas its small radius is between $B = 2.0$ and 2.4.

The free energy functional (3) is now discretized on an irregular lattice consisting of between 18744 and 26624 tetrahedron-like finite elements (depending on system size), which corresponds to 4892 up to 6848 vertices or, equivalently, to an average lattice constant of about 0.48. The tilt and twist angles are then defined on the vertices of the finite element grid and the total free energy is obtained numerically from an integration according to (3). (For further technical details on the finite element method for nematics we refer to the Appendix.) Starting from suitable initial configurations, the equilibrium director fields that correspond to local minima of the total free energy are calculated via a standard Newton-Gauß-Seidel relaxation method, where the director angles $\Theta_i$ and $\Phi_i$ on each internal vertex $i$ are immediately replaced by their respective corrected values, according to

$$
\Theta_i^{\text{new}} = \Theta_i^{\text{old}} - \frac{\partial F}{\partial \Theta_i} \quad \frac{\partial^2 F}{\partial \Theta_i^2} ,
$$

$$
\Phi_i^{\text{new}} = \Phi_i^{\text{old}} - \frac{\partial F}{\partial \Phi_i} \quad \frac{\partial^2 F}{\partial \Phi_i^2} .
$$

The functional derivatives in (4) and (5) are again evaluated numerically.

III. DIRECTOR CONFIGURATIONS IN A TORUS

Let us first introduce the different combinations of boundary and initial conditions as well as the external magnetic field. Both for homeotropic boundary conditions and for transversal-tangential anchoring, the following combinations of initial configurations and magnetic field direction are chosen: (a) a +1 ring defect with a homogeneous magnetic field along the $z$ axis, (b) both director and magnetic field homogeneous along $z$, (c) both director and magnetic field in azimuthal direction. Whereas (a) amounts in a distortion of the director field, (b) yields a topologically distinct configuration, consisting of two $+\frac{1}{2}$.
ring defects. (c) favors the “escape” of the director field along the azimuthal direction. For azimuthal-tangential anchoring we assume initial configurations with director and magnetic field along the $z$ and azimuthal direction, respectively. Finally, we consider a “laterally” homogeneous director and magnetic field, i.e., along the $x$ direction, as initial condition for several types of anchoring.

We start the discussion on director configurations in a toroidal volume by considering homeotropic surface anchoring. With the external magnetic field being switched off, there are mainly three possible solutions. Their visualization in the sections of the torus across the $x$-$z$ and $y$-$z$ coordinate planes is presented in Figure 3. If the director field does not exhibit an azimuthal component, there are closed disclinations, namely, defect rings. These rings can be classified according to the strength of the disclination \[33, 34\]. In our toroidal system we expect either one ring of strength $+1$ located in the central region of the torus (Fig. 3a) or, alternatively, two rings of strength $+\frac{1}{2}$ at its outer parts (Fig. 3b). Another possible director configuration is the “escape” structure (Fig. 3c) where the director in the bulk turns towards the azimuthal direction. In this way, the occurrence of defect rings would be suppressed.

For homeotropic anchoring, both the homogeneous magnetic field along $z$ and the azimuthal magnetic field are in conflict with the director orientation at the torus surface. The homogeneous field is expected to yield a ring configuration, whereas the azimuthal field favors the escape configuration. Figure 4 displays the energy of the three director configurations versus the inverse magnetic coherence length which, as indicated above, is proportional to the strength of the magnetic field. Please note that each of the three curves is related to the type of magnetic field favoring the respective bulk director orientation (see Figure caption for details). In order to compare systems of different size (the torus radii are $A = 7$, $B = 2$ and $A = 7$, $B = 2.4$ in the top and bottom part, respectively, of Figure 4) the total energy is divided by the torus volume $4\pi^2 AB^2$. Surprisingly, with zero magnetic field the escape structure is not stable. This is contrary to the director field in a cylindrical tube where disclinations are usually avoided by a director escape along the axis of the cylinder \[8, 10, 25, 26, 27\]. In a torus, however, the escape seems to be suppressed. Therefore, we attribute this behavior to the additional curvature along the azimuthal direction which is absent in a cylinder. Even when the small circle of the torus is increasing, the escape is far from being stable (Fig. 4, bottom). It can be stabilized against the global minimum only by
a strong magnetic field along the azimuthal direction which, for our parametrization, should correspond to a coherence length of at least 0.65.

From Figure 4 it is revealed that the global minimum configuration is the two-ring director field (Fig. 3b). Although the total topological charge is the same as in the one-ring configuration, it is energetically preferred, because a major percentage of the toroidal volume is filled by an almost homogeneous director field along $z$. (Obviously, the relative stability of the two-ring configuration is further enhanced by a homogeneous magnetic field along $z$.) Let us compare the situation to a spherical nematic drop subject to homeotropic surface anchoring. There, the analoga of the one-ring and two-ring configuration are a radial point defect [8, 9, 10, 11] and an equatorial defect ring (“Saturn ring”) [12, 13, 14, 15, 16, 17]. When the radius of the drop is not too small, the point defect is always favored to the ring, due to its much lower energy. In the torus, however, the two competing defect configurations are much more similar, and therefore it is the smooth director field rather than the defects which decides about their relative stability.

The situation is qualitatively changed for transversal-tangential surface anchoring. Again the one-ring, two-ring and escape configurations are possible solutions which are visualized in Figure 5. The one-ring configuration is known as closed vortex line (Fig. 5a), whereas the defects in the two-ring director field are located on the very surface of the torus (Fig. 5b). The escape configuration is analogous to the one for homeotropic anchoring (Fig. 5c). Interestingly, for not too large radii of the small circle of the torus and for weak magnetic fields, the escape is now absolutely stable (Fig. 6, top). A homogeneous magnetic field along $z$ with coherence length larger than 0.35 is needed to stabilize the closed vortex or surface defects against the escape. On the other hand, if we increase the small radius of the torus, the escape is suppressed again (Fig. 6, bottom). The stability of the escape for transversal-tangential anchoring can be understood from the elastic properties of the nematic sample. As stated, our parametrization is based on 5CB, which is an example for a rod-like molecule with elastic anisotropy $K_{33} > K_{11} > K_{22}$. The escape configuration with transversal-tangential anchoring mainly requires twist deformations, whereas for the escape with homeotropic anchoring bend deformations are predominant. For rod-like molecules, $K_{22}$ usually is the smallest elastic constant. Undergoing an escape, the increase of the elastic energy due to twist deformations is not too large, and it can be overcompensated by the disappearance of the defect rings. (For disc-like molecules the elastic anisotropy is re-
versed, which should cause a stable escape configuration in case of homeotropic rather than
tangential anchoring.)

As mentioned above, for increasing small radius of the torus, the escape becomes unstable
against the two-ring configuration. The latter enables an almost homogeneous director field
in the bulk, apart from the two closed surface disclinations. Here, the two-ring director field
is the analogon of the so-called “boojum” configuration in a spherical nematic drop with
tangential anchoring, where two point defects occur at opposite poles of the sphere [18, 19].

Whereas for homeotropic and transversal-tangential anchoring we find a smooth depen-
dence of the free energy on the strength of the magnetic field, the situation is different for
azimuthal-tangential anchoring. Obviously, an azimuthal director field now is the stable
configuration for zero magnetic field (Fig. 7a). When applying a homogeneous magnetic
field along $z$ (Fig. 7b), we find a threshold field strength which must be exceeded in order to
change the director configuration (Fig. 8). For magnetic fields slightly above the threshold
only the director in the central part of the torus turns into $z$ direction, which means an
abrupt jump of the energy to larger values. When the magnetic field further increases, the
director in the outer regions of the torus gradually aligns parallel to the magnetic field and,
therefore, the energy is again decreasing. As we notice from Figure 8, the threshold field
crucially depends on the small radius of the torus: for larger $B$ the onset of the reorientation
already occurs at smaller correlation lengths, mainly because the elastic deformation can be
spread over a larger region. On the other hand, the large radius $A$ of the torus does not
significantly influence the emerging director fields.

Finally, let us turn towards a more complicated scenario. When a strong homogeneous
magnetic field is applied along the $x$ direction, the system does not possess axial symmetry
any more. Therefore, we have to analyze the three-dimensional visualizations in detail.
We first consider a director configuration with homeotropic anchoring, subject to a lateral
magnetic field of reduced coherence length $\xi = 2.5$. This field is strong enough to force the
director in the bulk to align along $x$, which can clearly be seen from a top view onto the
section of the torus across the $x$-$y$ plane (Fig. 9, top). When we look at the sections across
the remaining coordinate planes (Fig. 9, bottom), two limits can be discerned in the director
alignment. Due to the director orientation in the bulk along $x$, locally in the $y$-$z$ plane there is
an escape, comparable to Figure 3c. On the other hand, the director configuration in the $x$-$z$
plane strongly resembles the two-ring configuration of Figure 3b, but with the disclinations
now appearing close to the upper and lower edge of the torus rather than in the \( x-y \) plane. Therefore, the fact that the escape configuration does not exhibit any defects means that the disclinations occurring in the \( x-z \) plane are curved, but not closed. Instead, they are of finite length, terminating at points where the bend deformation that causes the escape structure becomes more favorable energetically. Thereby, the extension of the disclinations covers an azimuthal range of \( \Delta \phi \approx \pi/3 \), as revealed from a more thorough analysis of the configuration.

An analogous director reorientation is observed for transversal-tangential anchoring (Fig. 10). Again, the escape structure occurs in the \( y-z \) plane, whereas in the \( x-z \) plane we now find the two-ring surface defects according to Fig. 5b. Here, these surface defects appear in the \( x-y \) plane (Fig. 10, bottom). Due to the smaller elastic splay energy, which dominates the reorientation in case of tangential anchoring, the escape covers a larger azimuthal range, thus reducing the extension of the surface defects to \( \Delta \phi \approx \pi/4 \).

IV. REMARKS

1. Summarizing our work, we have performed finite element calculations for director configurations of a nematic liquid crystal confined in a torus. Three different types of fixed surface anchoring, according to the toroidal geometry, were investigated. In addition, an external magnetic field was applied along directions forcing a reorientation of the director in the bulk. With zero magnetic field, the director “escape” along azimuthal direction turns out to be stable only for transversal-tangential anchoring. However, it is completely suppressed for homeotropic surface orientation where a configuration containing two defect rings is favored. For transversal-tangential anchoring these ring disclinations are located on the surface of the torus. When the surface anchoring is along the azimuthal direction, for a magnetic field applied along the symmetry axis of the torus, there is a threshold value which must be exceeded in order to force an abrupt reorientation of the bulk director.

2. Our three-dimensional finite element study allows the investigation of director configurations which are not any more axially symmetric. As an example we chose a scenario where a strong homogeneous magnetic field is applied laterally to the torus. The emerging director configuration turns out to contain both the “escape” along az-
imuthal direction and the disclinations, depending on the local azimuthal direction relative to the external magnetic field. The disclinations are curved, but of finite length, terminating at the intermediate regions where the energy gain due to the “escape” structure suppresses the formation of defects. Thereby, the extension of the disclinations depends on the type of surface anchoring.

3. The system of a nematic confined in a torus is the prototype of a complex geometry which, unlike nematic drops, is not any more simple connected. Finite element calculations in three dimensions is the appropriate technique to determine the equilibrium director configurations in such a system. Therefore, the results obtained can serve as a starting point for the investigation of more advanced scenarios, e.g., deformations of the confining torus or the presence of isotropic droplets immersed in the nematic.

APPENDIX A: FINITE ELEMENT TECHNIQUE FOR NEMATICS IN THREE DIMENSIONS

The method of finite elements is a means to minimize a functional defined on an arbitrarily complex geometry. In our case, this functional is the reduced elasto-magnetic free energy of a nematic liquid crystal (3), depending on the tilt and twist angle fields. We start by subdividing the toroidal volume into $L$ small tetrahedron-like finite elements. The total free energy is then expressed as the sum over the energy content of the $L$ finite elements, the director angles now being defined on the $N$ vertices of the grid. Each finite element has four corner vertices, thereby, the relation between elements and vertices is established by a neighbor list. Alltogether, this yields the discretized version of the reduced free energy (3),

$$ F[\Theta, \Phi] = \sum_{\alpha=1}^{L} F_\alpha \left[ \Theta_1^{(\alpha)}, \Theta_2^{(\alpha)}, \Theta_3^{(\alpha)}, \Theta_4^{(\alpha)}, \Phi_1^{(\alpha)}, \Phi_2^{(\alpha)}, \Phi_3^{(\alpha)}, \Phi_4^{(\alpha)} \right]. \quad (A1) $$

In (A1), the sum over $\alpha$ runs over all $L$ finite elements, $F_\alpha$ is the reduced free energy of the $\alpha$-th element. $\Theta_j^{(\alpha)}$ and $\Phi_j^{(\alpha)}$ are the director angles on the $j$-th corner vertex ($j = 1, 2, 3, 4$) of the $\alpha$-th element. For calculating $F_\alpha$, we introduce the Oseen-Zöcher-Frank free energy density $\overline{F}$, according to (3),

$$ \overline{F}_\alpha = \int_{V_\alpha} \text{d}^3x \overline{F}[\Theta(r), \Phi(r)]. \quad (A2) $$
Here, the integral is over the volume of the respective finite element. In order to unify the treatment of the finite elements, we apply a coordinate transformation from the vertex coordinates $x, y, z$ to natural coordinates $u, v, w$,

$$x^{(\alpha)} = x_1^{(\alpha)} + \left(x_2^{(\alpha)} - x_1^{(\alpha)}\right) u + \left(x_3^{(\alpha)} - x_1^{(\alpha)}\right) v + \left(x_4^{(\alpha)} - x_1^{(\alpha)}\right) w, \quad (A3)$$

$$y^{(\alpha)} = y_1^{(\alpha)} + \left(y_2^{(\alpha)} - y_1^{(\alpha)}\right) u + \left(y_3^{(\alpha)} - y_1^{(\alpha)}\right) v + \left(y_4^{(\alpha)} - y_1^{(\alpha)}\right) w, \quad (A4)$$

$$z^{(\alpha)} = z_1^{(\alpha)} + \left(z_2^{(\alpha)} - z_1^{(\alpha)}\right) u + \left(z_3^{(\alpha)} - z_1^{(\alpha)}\right) v + \left(z_4^{(\alpha)} - z_1^{(\alpha)}\right) w. \quad (A5)$$

In the transformations above, $x_j^{(\alpha)}, x_j^{(\alpha)} (j = 1, 2, 3, 4)$ are the cartesian coordinates of the $j$-th corner vertex of the $\alpha$-th finite element. In the new coordinates all finite elements are congruent. The free energy $F_\alpha$ now becomes

$$F_\alpha = \Delta_\alpha \int_0^1 d w \int_0^{1-w} d v \int_0^{1-v-w} d u \mathcal{F}[\Theta(u, v), \Phi(u, v)], \quad (A6)$$

with the Jacobian determinant $\Delta_\alpha$ of the coordinate transformation. When the grid is sufficiently fine, the director angle fields within one finite element can be approximated by a linear interpolation over the volume of the element,

$$\Theta^{(\alpha)} = \Theta_1^{(\alpha)} + \left(\Theta_2^{(\alpha)} - \Theta_1^{(\alpha)}\right) u + \left(\Theta_3^{(\alpha)} - \Theta_1^{(\alpha)}\right) v + \left(\Theta_4^{(\alpha)} - \Theta_1^{(\alpha)}\right) w, \quad (A7)$$

$$\Phi^{(\alpha)} = \Phi_1^{(\alpha)} + \left(\Phi_2^{(\alpha)} - \Phi_1^{(\alpha)}\right) u + \left(\Phi_3^{(\alpha)} - \Phi_1^{(\alpha)}\right) v + \left(\Phi_4^{(\alpha)} - \Phi_1^{(\alpha)}\right) w. \quad (A8)$$

After inserting (A7) and (A8) into (A6), due to the small size of the finite elements the integrand in (A6) is evaluated in the center of the finite element only. The integrals in (A6) then yield the product of the reduced free energy density $\mathcal{F}[\Theta^{(\alpha)}, \Phi^{(\alpha)}]$ and the volume of the finite element,

$$F_\alpha = \frac{1}{6} \Delta_\alpha \mathcal{F}[\Theta^{(\alpha)}, \Phi^{(\alpha)}]. \quad (A9)$$

In order to calculate the reduced free energy density $\mathcal{F}$, the director angles entering (3) are replaced by the respective averages of their values on the corner vertices. The partial derivatives occuring in (3) follow from the linear approximations (A7) and (A8).
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FIG. 1: Definition of the toroidal geometry. (a) Section across $x$-$z$ plane (side view), (b) section across $x$-$y$ plane (top view). The radii $A$ and $B$ denote the geometrical parameters of the confining torus.

FIG. 2: Fixed director field at the torus surface in sections across the $x$-$z$ and $y$-$z$ coordinate planes. (a) Homeotropic, (b) transversal-tangential, (c) azimuthal-tangential surface anchoring.

FIG. 4: Total energy $\vec{F}$ per volume of different director configurations vs. inverse magnetic coherence length $\xi$, for homeotropic surface anchoring. Squares: one-ring configuration, homogeneous magnetic field along $z$. $\times$-symbols: two-ring configuration, homogeneous magnetic field along $z$. Rhombs: escape configuration, azimuthal magnetic field. The upper and lower plots refer to the torus radii $A = 7$, $B = 2$ and $A = 7$, $B = 2.4$, respectively.

FIG. 5: Equilibrium director field in sections across the $x$-$z$ and $y$-$z$ coordinate planes for transversal-tangential surface anchoring. (a) One defect ring of topological strength +1 (vortex), (b) two surface defect rings of topological strength $+\frac{1}{2}$, (c) director “escape” along azimuthal direction.

FIG. 6: Total energy $\vec{F}$ per volume of different director configurations vs. inverse magnetic coherence length $\xi$, for transversal-tangential surface anchoring. Squares: one-ring configuration (vortex), homogeneous magnetic field along $z$. $\times$-symbols: two-ring configuration, homogeneous magnetic field along $z$. Rhombs: escape configuration, azimuthal magnetic field. The upper and lower plots refer to the torus radii $A = 7$, $B = 2$ and $A = 7$, $B = 2.4$, respectively.

FIG. 7: Equilibrium director field in sections across the $x$-$z$ and $y$-$z$ coordinate planes for azimuthal-tangential surface anchoring. (a) Azimuthal configuration below the magnetic threshold field, (b) distorted configuration above the magnetic threshold field.

FIG. 3: Equilibrium director field in sections across the $x$-$z$ and $y$-$z$ coordinate planes for homeotropic surface anchoring. (a) One defect ring of topological strength +1, (b) two defect rings of topological strength $+\frac{1}{2}$, (c) director “escape” along azimuthal direction.
FIG. 8: Total energy $\overline{F}$ per volume of the director field subject to a homogeneous magnetic field along $z$ vs. inverse magnetic coherence length $\overline{\xi}$, for azimuthal-tangential surface anchoring. Squares: torus radii $A = 7$, $B = 2$. $\times$-symbols: torus radii $A = 7$, $B = 2.4$.

FIG. 9: Equilibrium director field subject to a lateral homogeneous magnetic field along $x$ with inverse coherence length $\overline{\xi} = 2.5$, for homeotropic surface anchoring. (a) Section across the $x$-$y$ plane (top view), (b) sections across the $x$-$z$ and $y$-$z$ coordinate planes (oblique view).

FIG. 10: Equilibrium director field subject to a lateral homogeneous magnetic field along $x$ with inverse coherence length $\overline{\xi} = 2.5$, for transversal-tangential surface anchoring. (a) Section across the $x$-$y$ plane (top view), (b) sections across the $x$-$z$ and $y$-$z$ coordinate planes (oblique view).
J. Stelzer and R. Bernhard: Figure 1

(a)\[\begin{array}{c}
\text{z} \\
\hline \\
A \quad B
\end{array}\]

(b)\[\begin{array}{c}
\text{y} \\
\hline \\
A \quad B
\end{array}\]
(a) homeotropic

(b) transversal-tangential

(c) azimuthal-tangential
(a) one-ring configuration

(b) two-ring configuration

(c) escape configuration
J. Stelzer and R. Bernhard: Figure 4

In the figure, the total energy is plotted against the inverse magnetic coherence length for different reduced units. The energy values range from -0.3 to 0.4, while the inverse magnetic coherence length varies from 0 to 1.
(a) one-ring configuration

(b) two-ring configuration

(c) escape configuration
total energy [reduced units]

inverse magnetic coherence length [reduced units]
(a) below threshold

(b) above threshold
J. Stelzer and R. Bernhard : Figure 8

inverse magnetic coherence length
[reduced units]
(a) top view

(b) oblique view
(a) top view

(b) oblique view