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EQUILIBRIUM CONFIGURATIONS OF NEMATIC LIQUID CRYSTALS ON A TORUS

ANTONIO SEGATTI, MICHAEL SNARSKI, AND MARCO VENERONI

Abstract. The topology and the geometry of a surface play a fundamental role in determining the equilibrium configurations of thin films of liquid crystals. We propose here a theoretical analysis of a recently introduced surface Frank energy, in the case of two-dimensional nematic liquid crystals coating a toroidal particle. Our aim is to show how a different modeling of the effect of extrinsic curvature acts as a selection principle among equilibria of the classical energy, and how new configurations emerge. In particular, our analysis predicts the existence of new stable equilibria with complex windings.

Due to their special optical properties and their controllability through electric and magnetic fields, liquid crystals have proven to be fundamental in many scientific and technological applications. Their properties have been deeply investigated for over a century and nowadays increasing emphasis is being placed on so-called nematic shells. These are microscopic particles coated by a thin film of liquid crystals, which develop defects with a topological charge, and thus have a tendency to self-assemble into metamaterials which may have new optical properties and a high potential for technological applications (see, e.g., [14, 22]). The form of the elastic energy for nematics is well established, both in the framework of director theory, based on the works of Oseen, Zocher, and Frank, and in the framework of the order-tensor theory introduced by de Gennes (see, e.g., [20, 3, 18]). In contrast, there is no universal agreement on the *two-dimensional* free energy to model nematic shells. Different ways to take into account the distorsion effect of the substrate were proposed in [19, 7, 9] and recently by Napoli and Vergori ([12, 11]). Indeed, as observed in [21] and [1], the liquid crystal ground state (and all its stable configurations, in general) is the result of the competition between two driving principles: on one hand the minimization of the "curvature of the texture" penalized by the elastic energy, and on the other the frustration due to constraints of geometrical and topological nature, imposed by anchoring the nematic to the surface of the underlying particle. The new energy model ([12, 11]) affects these two aspects, focusing on the effects of the extrinsic geometry of the substrate on the elastic energy of the nematics. With the present Letter we aim at exploring the full consequences of the new model so that a detailed comparison with the classical one can be established. More precisely, we study the two- dimensional Napoli-Vergori director theory for nematic shells on a genus one surface: *a)* we analyze the dependence of the new energy on the mechanical parameters (splay, twist and bend moduli) and on the geometrical parameters (the radii of the torus); *b)* we highlight in which cases the new energy acts as a *selection principle* among the minimizers of the classical one, and in which cases *new* different states emerge; *c)* we predict the existence of stable equilibrium states carrying a higher energy than the ground state, in correspondence with the homotopy classes of the torus. Our analysis, in particular, agrees and makes more

precise the statement of [11], according to which the new energy "promotes the alignment of the flux lines of the nematic director towards geodesics and/ or lines of curvature of the surface". The aspect of high energy equilibrium states is present in the classical energy as well, but it was neglected in previous research on genus one surfaces ([9]).

Our observations are based on a rigorous mathematical analysis of the models, which combines methods from differential geometry and topology, calculus of variations, functional analysis and numerical simulations. Topology enters our work, first of all, in the choice of the torus as base substrate. Indeed the nematics would necessarily present defects on any surface with genus different than one, due to Poincaré-Hopf Theorem ([13, 10, 9]); as a consequence, when dealing with the Frank's director theory, the space of functions in which one looks for minimizers would be empty, even in a weak sense (see [2]), requiring thus further expedients or approximations (see, e.g., [17, 21]). In order to focus on the influence of the geometry, we choose a surface where defectless ground states can be found. The case of a cylinder, the simplest surface where different results between classical and new energy can be predicted, was presented in [11] (on a sphere, the two energies differ by a constant). A related energy on hyperbolic surfaces was studied in [5]. Although the experimental generation of toroidal nematics is a challenge, recent techniques ([16]) allow for droplets of genus one or higher, and further motivate investigation of more complex surfaces.

In the classical director theory of nematics, the local orientation of the liquid crystal molecules in a sample $\Omega \subset \mathbb{R}^3$ is described by the unit vector field $\mathbf{n} : \Omega \to \mathbb{S}^2$, where $\mathbb{S}^2$ is the unit sphere. Stable configurations are minimizers of the classical elastic energy, which according to Frank's formula reads

$$\begin{aligned} W(\mathbf{n}) := \frac{1}{2}\int_\Omega \big[& K_1(\operatorname{div}\mathbf{n})^2 + K_2(\mathbf{n}\cdot\operatorname{curl}\mathbf{n})^2 \\ & + K_3|\mathbf{n}\times\operatorname{curl}\mathbf{n}|^2 \\ & + (K_2+K_{24})\operatorname{div}\left[(\nabla\mathbf{n})\mathbf{n} - (\operatorname{div}\mathbf{n})\mathbf{n}\right]\big]\,\mathrm{d}x, \end{aligned}$$

where K_1, K_2, K_3 and K_{24} are positive constants called the splay, twist, bend and saddle-splay moduli, respectively. The last term is a null Lagrangian, hence it depends only on the behavior of $\mathbf{n}$ on the boundary. While the Frank's energy above is, within the director theories, well accepted, there is not such agreement when dealing with surface energies. In the literature, one can find different proposals for such an energy ([19, 9, 21] [11]). The main difference between the classical energy proposed in [19, 9, 21] and the most recent one [11] essentially lies in the choice of the differential operators on the surface S. More precisely, the energy in ([19, 9, 21]) is a functional of the covariant derivative $D\mathbf{n}$ of the vector field $\mathbf{n}$, while the energy in [11] depends on the surface gradient $\nabla_s\mathbf{n}$, which is defined as $\nabla_s\mathbf{n} := \nabla\mathbf{n}P$ (see, e.g., [20]), with P being the orthogonal projection onto the tangent plane of S. In other words, ∇_s is the restriction of the usual derivative of $\mathbb{R}^3$ to directions lying in the tangent plane and takes thus into account also the extrinsic curvature of S. In order to describe the elastic energy of a thin film, approximated by a surface S, we resort to the Darboux frame $\{\mathbf{n}, \mathbf{t}, \boldsymbol{\nu}\}$, where $\boldsymbol{\nu}$ is the unit normal vector to S and $\mathbf{t} := \boldsymbol{\nu}\times\mathbf{n}$. Let $\kappa_\mathbf{t}, \kappa_\mathbf{n}$ be the geodesic curvatures of the flux lines of $\mathbf{t}$ and $\mathbf{n}$, respectively. Let $c_\mathbf{n}$ be the normal curvature and let $\tau_\mathbf{n}$ be the geodesic torsion (see, e.g., [4] for all the definitions and examples related to differential geometry). The

surface divergence acting on the field $\mathbf{n}$ is defined as $\mathrm{div}_s\mathbf{n} := \mathrm{tr}D\mathbf{n} = \mathrm{tr}\nabla_s\mathbf{n}$ and can be expressed as $\mathrm{div}_s\mathbf{n} = \kappa_{\mathbf{t}}$ ([11]). The classical form of surface free energy, for a thin film of nematics of constant thickness h around S, is ([19, 9, 21])

$$\begin{aligned} W_{\mathrm{Cl}}(\mathbf{n}) &:= \frac{1}{2}\int_S \left[k_1(\mathrm{div}_s\mathbf{n})^2 + k_3(\mathrm{curl}\,\mathbf{n})^2\right] \mathrm{d}A, \\ &= \frac{1}{2}\int_S \left[k_1\kappa_{\mathbf{t}}^2 + k_3\kappa_{\mathbf{n}}^2\right] \mathrm{d}A, \end{aligned} \tag{1}$$

where $k_i = hK_i$ and $\mathrm{curl}\,\mathbf{n}$ is the covariant curl operator (see [8]). In the new energy introduced in [11], the extrinsic curvature of S comes to play a role through $c_{\mathbf{n}}$ and $\tau_{\mathbf{n}}$

$$\begin{aligned} W_{\mathrm{NV}}(\mathbf{n}) &:= \frac{1}{2}\int_S \left[k_1(\mathrm{div}_s\mathbf{n})^2 + k_2(\mathbf{n}\cdot\mathrm{curl}_s\mathbf{n})^2\right. \\ &\qquad \left. + k_3|\mathbf{n}\times\mathrm{curl}_s\mathbf{n}|^2\right] \mathrm{d}A, \\ &= \frac{1}{2}\int_S \left[k_1\kappa_{\mathbf{t}}^2 + k_2\tau_{\mathbf{n}}^2 + k_3(\kappa_{\mathbf{n}}^2 + c_{\mathbf{n}}^2)\right] \mathrm{d}A, \end{aligned} \tag{2}$$

where $\mathrm{curl}_s\mathbf{n} := -\epsilon\nabla_s\mathbf{n}$ (ϵ is the Ricci alternator). Note that $\mathrm{curl}_s\mathbf{n} = -\tau_{\mathbf{n}}\mathbf{n} - c_{\mathbf{n}}\mathbf{t} + \kappa_{\mathbf{n}}\boldsymbol{\nu}$ and that, unless we restrict to flat surfaces, the vector $\mathrm{curl}_s\mathbf{n}$ has non vanishing in-plane components. Note also that the saddle-splay term is not present in the surface energy W_{NV} (see [11] for a justification). In order to study the minimizers of W_{Cl} and W_{NV}, it is convenient to introduce a parametrization X of S. We use (θ,ϕ) as a set of local coordinates and we assume that $\mathbf{e}_\theta := \partial_\theta X/|\partial_\theta X|$ and $\mathbf{e}_\phi := \partial_\phi X/|\partial_\phi X|$ give a local orthonormal basis for the tangent plane to S. We can then describe $\mathbf{n}$ through the angle α defined by $\mathbf{n} = \mathbf{e}_\theta\cos\alpha + \mathbf{e}_\phi\sin\alpha$. With respect to α, the surface energy (2) takes the form

$$\begin{aligned} W_{\mathrm{NV}}(\alpha) = \frac{1}{2}\int_S &\left[k_1((\nabla_s\alpha - \boldsymbol{\Omega})\cdot\mathbf{t})^2 + k_3((\nabla_s\alpha - \boldsymbol{\Omega})\cdot\mathbf{n})^2\right. \\ &+ k_2(c_1-c_2)^2\sin^2\alpha\cos^2\alpha \\ &\left.+k_3(c_1\cos^2\alpha + c_2\sin^2\alpha)^2\right] \mathrm{d}A, \end{aligned}$$

where c_1 and c_2 are the principal curvatures of S and $\boldsymbol{\Omega}$ is the spin connection (see [15]). The first two terms coincide with W_{Cl}.

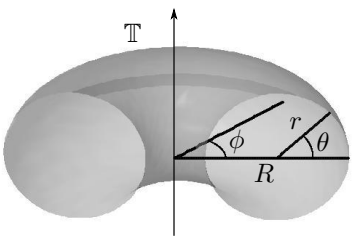


FIGURE 1. Schematic representation of the torus $\mathbb{T}$.

We now focus on the case of a torus $\mathbb{T}$, with radii $R > r > 0$ (see Figure 1), parametrized by

$$X(\theta, \phi) = \begin{pmatrix} (R + r\cos\theta)\cos\phi \\ (R + r\cos\theta)\sin\phi \\ r\sin\theta \end{pmatrix}, \tag{3}$$

where $(\theta, \phi) \in Q := [0, 2\pi] \times [0, 2\pi]$. In order to study the dependence of the energy (2) on the mechanical and geometrical parameters, we first restrict to the case of *constant angle* α. In this case, the integral in (2) can be computed explicitly as a function of five real parameters:

$$\begin{aligned} W_{\mathrm{NV}} &= W_{\mathrm{NV}}(\alpha, k_1, k_2, k_3, \mu) \\ &= 2\pi^2 \left(k_1 \cos^2\alpha + k_3 \sin^2\alpha\right) \left(\mu - \sqrt{\mu^2 - 1}\right) \\ &\quad + \frac{\pi^2}{2} \left(k_2 \sin^2(2\alpha) + k_3 \cos^2(2\alpha)\right) \frac{\mu^2}{\sqrt{\mu^2 - 1}} \\ &\quad + \pi^2 k_3 \cos(2\alpha) \left(2\mu - \frac{\mu^2}{\sqrt{\mu^2 - 1}}\right) + \frac{\pi^2 k_3 \mu^2}{2\sqrt{\mu^2 - 1}}, \end{aligned}$$

where $\mu := R/r$. We note that the last term, which is independent of α, is the value of Helfrich's functional ([6]) on the torus characterized by the ratio μ (and zero spontaneous curvature). Since W_{NV} is π-periodic, we restrict to $\alpha \in]-\pi/2, \pi/2]$.

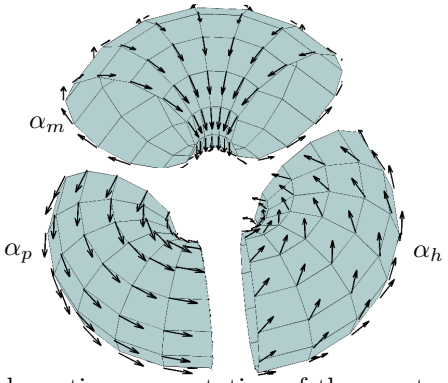


FIGURE 2. Schematic representation of the constant equilibrium configurations α_m, α_p and α_h, where the director field $\mathbf{n}$ is aligned along meridians, parallels and helixes of $\mathbb{T}$, respectively.

Studying the equilibrium equation associated with W_{NV}, one finds the equilibrium configurations (see Figure 2)

$$\alpha_m = 0, \quad \alpha_p = \frac{\pi}{2}, \quad \alpha_h = \pm\frac{1}{2} \arccos\left(\frac{Bk_3 + Ck_1}{\mu^2(k_2 - k_3)}\right),$$

where $B = \mu\sqrt{\mu^2 - 1} - 1$ and $C = B - \mu^2 + 2$ (provided that the argument of the arccos function is in the interval $[-1, 1]$).

The explicit form of W_{NV} actually allows for a complete study which is beyond the scope of this note, so we conclude this part with a remark. Unlike the case of the cylinder [11], the minimality depends also on the ratio $\mu = R/r$. In this regard,

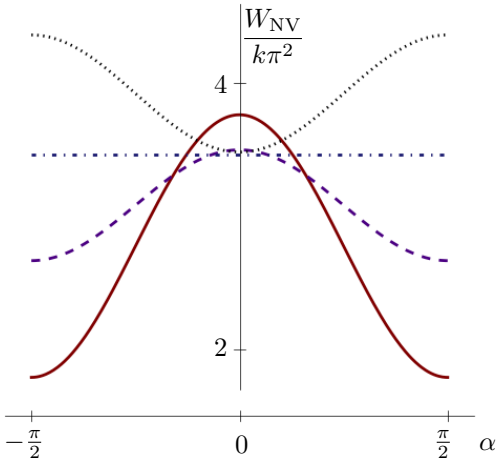


FIGURE 3. Surface energy W_{NV} (rescaled by $k\pi^2$) as a function of the deviation α from $\mathbf{e}_\theta$, for the one-constant approximation $k := k_1 = k_2 = k_3$. The ratio of the radii of the torus $\mu = R/r$ is : $\mu = 1.1$ (dotted line), $\mu = 2/\sqrt{3}$ (dashed dotted line), $R/r = 1.25$ (dashed line), $R/r = 1.6$ (continuous line). The behavior for equal k_j's depends on the fact that the only non-constant term in the energy W_{NV} changes sign when $2\mu = \mu^2/\sqrt{\mu^2 - 1}$, i.e. when $\mu = 2/\sqrt{3}$.

see Figure 3, where $W_{\mathrm{NV}}(\alpha)$ is plotted for fixed k_j and different choices of μ, and Figure 4, which shows $W_{\mathrm{NV}}(\alpha)$ for fixed ratio μ and different choices of k_j.

We turn now our attention to *general* functions α (i.e., not necessarily constants), in the case of the well-studied one-constant approximation of W_{NV}, where $k_1 = k_2 = k_3 =: k$. Let $\nabla_s \mathbf{n}$ be the surface derivative of $\mathbf{n}$ and let $\boldsymbol{\nu}$ be the unit normal vector to the torus $\mathbb{T}$; the role of the extrinsic curvature of $\mathbb{T}$ on the free energy can clearly be seen from the orthogonal decomposition $\nabla_s \mathbf{n} = D\mathbf{n} - \boldsymbol{\nu} \otimes (\nabla_s \boldsymbol{\nu})\mathbf{n}$, recalling that $-\nabla_s \boldsymbol{\nu}$ is the extrinsic curvature tensor (see [4]). The one-constant approximation of W_{NV} is then

$$W_{\mathrm{NV}}(\mathbf{n}) = \frac{k}{2} \int_{\mathbb{T}} |\nabla_s \mathbf{n}|^2 \mathrm{d}A,$$

or, in terms of the angle α with the local coordinates,

$$W_{\mathrm{NV}}(\alpha) = f(\mu) + \frac{k}{2} \int_{\mathbb{T}} \left[|\nabla_s \alpha|^2 + \frac{c_1^2 - c_2^2}{2} \cos(2\alpha) \right] \mathrm{d}A,$$

where $f(\mu) = \kappa\pi^2(2\mu + (2-\mu^2)/\sqrt{\mu^2 - 1}))$ can be computed using the orthogonality of $\nabla_s \alpha$ and $\boldsymbol{\Omega}$. The corresponding Euler-Lagrange equation is

$$k\Delta_s \alpha + \frac{k}{2}(c_1^2 - c_2^2)\sin(2\alpha) = 0, \tag{4}$$

where $\Delta_s = \mathrm{div}_s \nabla_s$ is the Laplace-Beltrami operator on the torus $\mathbb{T}$. Equation (4) is a novel kind of elliptic sine- Gordon equation, the only explicit solutions to which, to our knowledge, are the constants $\alpha_m = 0$ and $\alpha_p = \pi/2$. We resort thus to studying the gradient flow of W_{NV}, i.e., the solutions $\alpha = \alpha(x, t)$ defined on

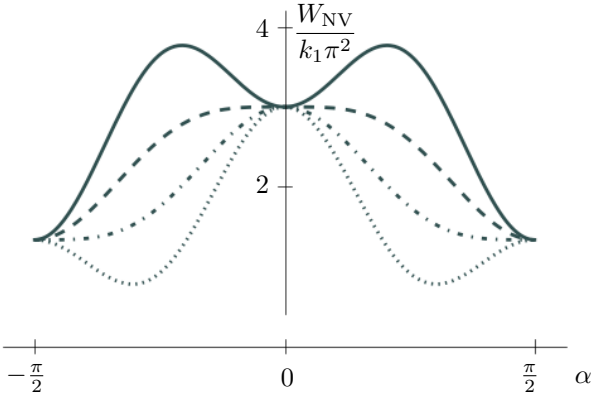


FIGURE 4. Surface energy W_{NV} (rescaled by $k_1\pi^2$) as a function of the deviation α from $\mathbf{e}_\theta$, for $\mu = 1.25$, $k_1 = k_3 = 1$ and different values of k_2. Studying the second derivative of W_{NV}, one finds critical values $\xi_1 = 2\sqrt{\mu^2-1}/\mu$ and $\xi_2 = 2-\xi_1$, which characterize the cases: α_m is local minimum and α_p is global minimum ($k_2 > \xi_1$, continuous line); α_m is global maximum and α_p is global minimum ($\xi_1 \geq k_2 \geq \xi_2$, between dashed and dashed-dotted lines); $\pm\alpha_h$ are global minima, α_p is local maximum, α_m is global maximum ($k_2 < \xi_2$, dotted line).

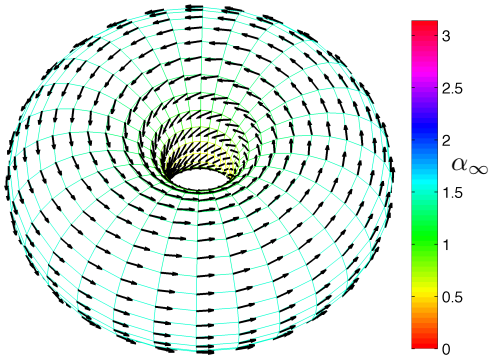
$\mathbb{T} \times [0, +\infty)$, to the evolution equation

$$\partial_t \alpha = k\Delta_s \alpha + \frac{k}{2}(c_1^2 - c_2^2)\sin(2\alpha), \tag{5}$$

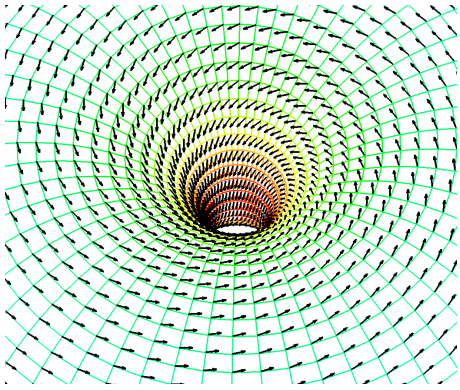
equipped with an initial datum $\alpha(x, 0) = \alpha_0(x)$ on $\mathbb{T}$. We remark that this evolution problem is not a physical flow of the nematics, but it constitutes an efficient mathematical artifice to approximate solutions of the stationary equation (4). Indeed, owing to the ellipticity of the Laplace-Beltrami operator and to the regularity of the nonlinear term, for any regular initial datum α_0 there exists a unique solution $\alpha(t)$ to (5). Moreover, by construction, at any time $t > 0$ this solution satisfies the energy balance

$$\int_0^t \int_{\mathbb{T}} |\partial_t \alpha(s)|^2 \mathrm{d}A\, \mathrm{d}s + W_{\mathrm{NV}}(\alpha(t)) = W_{\mathrm{NV}}(\alpha_0),$$

which implies that $t \mapsto W_{\mathrm{NV}}(\alpha(t))$ is monotone decreasing. Finally, as $t \to +\infty$, $\alpha(t)$ converges (possibly up to a subsequence) to a function α_∞ which solves (4). If α_0 is a critical point, i.e. $\alpha_0 = \alpha_m$ or $\alpha_0 = \alpha_p$, then the evolution is clearly constant: $\alpha(t) \equiv \alpha_m$, or $\alpha(t) \equiv \alpha_p$, respectively. (Color online) For different initial data, we find as a limit solution either α_p, or a nonconstant α_∞ belonging to the family illustrated in Figure 5. The only distinguishing factor between these two behaviors is the ratio of radii R/r. From the explicit form of $W_{\mathrm{NV}}(\alpha)$, we know that if $\mu \geq 2$, then $c_1^2 - c_2^2 \geq 0$ and thus $\alpha_p \equiv \pi/2$ is the unique (up to rotations of $m\pi, m \in \mathbb{Z}$) global minimizer of W_{NV}. On the other hand, from the previous discussion on constant α, we know that if $\mu < 2/\sqrt{3}$, then α_p cannot be the global minimizer, as for this ratio $W_{\mathrm{NV}}(\alpha_m) < W_{\mathrm{NV}}(\alpha_p)$. We conjecture that there exists



a) $\mu = 1.4$



b) $\mu = 1.2$

FIGURE 5. Plots of the vector field $\mathbf{n}_\infty$ corresponding to the limit solution α_∞ to (5) for $\alpha_0 = \pi/4$ and different ratios μ. (The color code represents α_∞.) For $\mu < 2$, the configuration α_m is preferable in a strip close to the central hole, while for every choice of μ, α_p is more convenient around the external equator. As the term $|\nabla_s \alpha|^2$ in the energy penalizes the transition from α_p to α_m, minimizers exhibit a smooth rotation of the director field along the meridians. The amplitude of the rotation increases as μ decreases to 1.

a unique critical ratio $\mu^* \in (2/\sqrt{3}, 2)$ above which α_p is the point of minimum, and below which the nonconstant solution appears. Numerically, we found $\mu^* \sim 1.52$.

It is interesting to compare these configurations with the equilibrium ones of the classical Frank energy [9]. In the one-constant approximation, the energy on a torus is

$$\begin{aligned} W_{\mathrm{Cl}}(\alpha) &= \frac{k}{2} \int_{\mathbb{T}} |\nabla_s \alpha - \mathbf{\Omega}|^2 \, \mathrm{d}A \\ &= \frac{k}{2} \int_{\mathbb{T}} |\nabla_s \alpha|^2 \, \mathrm{d}A + 2k\pi^2(\mu - \sqrt{\mu^2 - 1}) \end{aligned}$$

and the corresponding equilibrium equation is $\Delta_s \alpha = 0$. (Note that in [9] $\mu = r/R$.) Therefore, in the classical case, every field $\mathbf{n} = \mathbf{e}_\theta \cos\bar{\alpha} + \mathbf{e}_\phi \sin\bar{\alpha}$, for constant $\bar{\alpha}$, is

an equilibrium state, with the same energy independently of $\bar{\alpha}$. For $\mu > \mu^*$, the new energy W_{NV} selects α_p, among all constants, as unique equilibrium configuration. For $\mu < \mu^*$, instead, the new lower- energy configuration shown in Figure 5 appears.

In order to describe more complex equilibrium states, we need to introduce the winding number of the director field $\mathbf{n}$ on the torus. Let $\mathbf{n}$ be given and, referring to (3), let $\alpha : Q \to \mathbb{R}$ be such that

$$\mathbf{n}(X) = \mathbf{e}_\theta \cos\alpha + \mathbf{e}_\phi \sin\alpha \quad \text{on } Q.$$

Though α needs not be Q-periodic, there certainly exist, since $\mathbf{n}$ is continuous, integers $m, n \in \mathbb{Z}$ such that

$$\alpha(2\pi, 0) = \alpha(0,0) + 2m\pi, \qquad \alpha(0, 2\pi) = \alpha(0,0) + 2n\pi.$$

We define the *winding number* of $\mathbf{n}$ as the couple of indices $\mathbf{h} = (h_\theta, h_\phi) \in \mathbb{Z} \times \mathbb{Z}$, given by

$$h_\theta := \frac{\alpha(2\pi,0) - \alpha(0,0)}{2\pi}, \qquad h_\phi := \frac{\alpha(0,2\pi) - \alpha(0,0)}{2\pi}.$$

Geometrically, h_θ indicates how many full turns of 360° are completed by $\mathbf{n}$ along the meridian line parametrized by $\theta \mapsto X(\theta, 0)$; similarly, the number of turns along the parallel line $\phi \mapsto X(0,\phi)$ is given by h_ϕ. A crucial property of the winding number is its invariance under continuous transformations of the field $\mathbf{n}$ (so that $\mathbf{h}$ could be equivalently computed on any pair of curves which are homotopically equivalent to the two that we chose). The relevant consequence is the following: for any choice of $\mathbf{h} = (h_\theta, h_\phi) \in \mathbb{Z} \times \mathbb{Z}$, there is an initial datum α_0 (e.g., $\alpha_0(\theta,\phi) = h_\theta\theta + h_\phi\phi$) such that the corresponding vector field $\mathbf{n}$ has winding number $\mathbf{h}$; the evolution of α_0 according to (5) provides then, in the limit as $t \to +\infty$, a function α_∞ whose associated vector field $\mathbf{n}_\infty$ is a local minimizer of W_{NV}, and has winding number $\mathbf{h}$. There exists therefore at least one equilibrium configuration for each choice of winding number, and this configuration is stable, in the sense that it is not possible to lower its energy without breaking the pattern on a line, i.e., without creating a line defect. Nonetheless, as the elastic energy increases monotonically with $|\mathbf{h}|$, we expect the existence of an upper bound on the observable winding number of the nematics field, depending on the maximum elastic energy that the specific liquid crystal can undergo before breaking.

In conclusion, we analyzed nematic liquid crystals on a toroidal particle, finding new equilibrium configurations for the surface energy recently proposed by Napoli and Vergori in [12, 11] and comparing them to the equilibria of classical energies. We identified a range of parameters where the new energy selects a unique equilibrium among the classical ones, and we showed the emergence of new equilibria configurations, in accordance with the new penalization of the normal curvature and geodesic torsion of the director field. We hope that experiments could be carried out in order to confirm our analysis.

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