ANALYSIS OF A MODEL FOR BENT-CORE LIQUID CRYSTALS COLUMNAR PHASES

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Abstract. We consider a model originally introduced to study layer-undulated structures in bent-core molecule liquid crystals. We first prove existence of minimizers, then analyze a simplified version used to study how in columnar phases the width of the column affects the type of switching, which occurs under an applied electric field. We show via Γ-convergence that as the width of the column tends to infinity, rotation around the tilt cone is favored, provided the coefficient of the coupling term, between the polar parameter, the nematic parameter, and the layer normal is large.

1. Introduction. Bent-core molecule liquid crystals (BLCs) are achiral molecule materials, which exhibit phases typical of chiral liquid crystals (LCs). Due to this characteristic, they have been in recent years the subject of a noticeable amount of theoretical and experimental work in the physics community, see [7, 2013] for a review of the available literature on BLCs. Among other approaches, phenomenological Landau models have been successfully employed to analyze and numerically approximate the smectic behavior of these amazingly phase-rich materials.

The main focus of this paper is a version, presented in [8, 2005], of the free energy first introduced by Vaupotić and Ćopić in [16, 2005]. Vaupotić and Ćopić’s interest in [16] lies on the polarization-modulated layer-undulated structure found in some tilted smectic phases, and the key feature of their model is the coupling term between the polarization splay and the tilt of the material molecules with respect to the normal vector of the smectic layers. In [8], instead the authors look at the type of switching under applied electric field encountered in the so-called columnar phases, where the material forms two-dimensional structures made of fragments of smectic layers, which is seen experimentally in BLCs.

We first introduce a slight modification of the full energy functional proposed in [16], needed to guarantee mathematical well-posedness, and prove existence of minimizers. We then set up the mathematical framework to study the reduced functional considered in [8]. These are inherently one-dimensional problems, which nevertheless are of mathematical interest as the two unknown functions describing...
the state of the BLC are mutually orthogonal unit vectors. We use $\Gamma$-convergence to derive a limiting energy functional for the large-column width case, and argue that there are only two candidates for minimizers of the limiting functional, which respectively represent switching by rotation on the tilt cone, and along the axis of the molecule, see Remark 2. We obtain some basic estimates to show that the state representing switching by rotation on the tilt cone is in this limiting case the minimizer for certain values of the physical parameters.

The paper is organized as follows. In Section 2, we introduced the relevant terminology, and provide some background to illustrate the physical picture underlying the problem. We present in Section 3 the full version of the model, suitably modified, and we show existence of minimizers. Section 4 is devoted to the study of columnar phases in the case of large columnar width. In Section 5, we study the minimizers of the $\Gamma$-limit energy and obtain some simple energy estimates, which are functions of the physical parameters.

2. Background. In a very simplified illustration, we think to temperature as providing a measure of random motion, with its increase affecting the ability of attractive intermolecular forces to keep order. Solids can be then pictured as regularly stacked molecules having positional and orientational order, and liquids as molecules free to randomly move, with no positional or orientational order. For thermotropic liquid crystals, the transition from crystalline states to isotropic liquid states, which is induced by varying temperature, is characterized by in between thermodynamically anisotropic fluid-like stable phases. In these in between phases, liquid crystals may retain some of the mechanical properties of fluids, but more importantly they retain some of the optical features of crystals, hence their use and importance in the manufacturing of display devices. Figure 1 provides a standard simple microscopic picture of this behavior, which originates from the fact that many LC materials have rod-like (strongly elongated in one direction) molecules. The key point to keep in mind is that in a liquid crystalline phase some positional or all order may be lost,
but some orientational order remains, and one can define a preferred local average direction, represented by a unit vector, \( \mathbf{n} \), called the director, see inset of Figure 1.

The liquid crystalline phases are grossly divided in two families: nematic and smectic. The nematic phase, N, is distinguished by the presence of some degree of long-range orientational order, but no positional order. The molecules can be polar but the states described by \( \mathbf{n} \) and \(-\mathbf{n}\) are physically the same. The director in the variation chiral nematic phase, \( \mathrm{N}^* \), rotates in a helical sense throughout the sample, see Figure 2.

The smectic phases manifest also a small amount of orientational order, but now also some degree of positional order is present: the molecules are arranged on average in equidistant planes, and one has a layered structure with a well-defined interlayer spacing. The smectic layer normal is denoted by \( \mathbf{\nu} \). Two common smectic phases are the smectic A (SmA), and the smectic C (SmC), with their chiral variants, SmA* and SmC*. In the SmA phase, the axes of orientational and positional order are parallel, while in the SmC phase orientational and positional orders are tilted one with respect to the other, see inset of Figure 1, and so the director \( \mathbf{n} \) is tilted at a defined angle, the tilted angle \( \theta \), to the layer normal \( \mathbf{\nu} \). In general, the tilt magnitude \( \theta \) is well-defined at given values of pressure and temperature, while the azimuthal or phase angle \( \phi \) is not, and \( \mathbf{n} \) is located somewhere on the cone of axis \( \mathbf{\nu} \) and opening angle \( \theta \), called the tilt cone. The chiral SmC* phase is characterized by an helical superstructure, the helix axis is along \( \mathbf{\nu} \) while the azimuthal angle \( \phi \) is the quantity changing when proceeding along the axis, see Figure 2.

![Figure 2. Schematic of chiral phases.](image)

The SmC* is a particularly interesting phase in soft matter, since chirality has significant consequences, which include the appearance of a (mesoscopic) electric polarization. In this phase the polarization is parallel to \( \mathbf{n} \times \mathbf{\nu} \), and it too changes direction as \( \mathbf{n} \) travels along the helical axis, thus typically, the macroscopic polarization is zero. Nevertheless, under proper manipulation some LCs can exhibit ferroelectric behavior, which is of great interest for technological applications. Usually, a LC which displays this phase has chiral molecules, that is molecules that differ from their mirror image, but still have no head or tail. Recently it was discovered that macroscopically chiral smectic phases are observed in certain achiral compounds, where the bent geometry of the molecules gives rise to a polar order.
perpendicular to the molecular axis, see Figure 3. Cost efficiency manufacturing considerations, and richness in the variety of phases observed, have made these materials the subject of many theoretical and experimental physical studies, [7]. The mathematical treatments are nevertheless still very scant, although validation and analysis of the available models might result in new relevant contributions to the area, see for example [3].

Bent-core molecule liquid crystals, schematically depicted in Figure 3, have a characteristic banana shape, and can be described by the tilt angle $\theta$, the azimuthal angle $\phi$, the layer tilt angle $\Delta$, and the polar angle $\alpha$, [16, 3]. We will use the following convention for these fundamental angles. We take the layer tilt angle $\Delta$ to be defined modulo $2\pi$ as the angle from the $z$-axis toward the $x$-axis about the positive $y$-axis, with this choice the layer normal is given by $\mathbf{nu} = \langle \sin \Delta, 0, \cos \Delta \rangle$.

The tilt angle $\theta$ is the angle between $\mathbf{n}$ and $\mathbf{nu}$, that is $\mathbf{n} \cdot \mathbf{nu} = \cos \theta$, and has values $0 \leq \theta \leq \pi$. We define the azimuthal angle $\phi$ as the angle from $\mathbf{t}$ toward $\mathbf{s}$ about $\mathbf{nu}$, where $\mathbf{t}$ is the unit vector in the $x$-$z$ plane perpendicular to $\mathbf{nu}$, and such that $\mathbf{t} \times \mathbf{nu}$ is in the negative $y$ direction; while $\mathbf{s}$ is a unit vector in the $\mathbf{nu}$-$\mathbf{n}$ plane, perpendicular to $\mathbf{nu}$ and such that $\mathbf{t} \times \mathbf{nu}$ is in the same direction as $\mathbf{n} \times \mathbf{nu}$. Finally, the polar angle $\alpha$ is the angle obtained from $\mathbf{n} \times \mathbf{nu}$ to $\mathbf{p}$ about $\mathbf{n}$, with $\alpha \in (-\pi, \pi)$. Note that $\alpha$ and $\phi$ are not defined if $\mathbf{n}$ and $\mathbf{nu}$ are parallel, in this work, when using this representation, we will always assume that $\theta \neq 0, \pi$. We can write the layer normal, and the nematic and polar directors in terms of the molecular angles as follows:

$$
\mathbf{nu} = \langle \sin \Delta, 0, \cos \Delta \rangle;
$$

$$
\mathbf{n} = \langle \sin \Delta \cos \theta + \sin \theta \cos \phi \cos \Delta, \\
\sin \theta \sin \phi, \cos \theta \cos \Delta - \sin \theta \sin \Delta \cos \phi \rangle;
$$

$$
\mathbf{p} = \langle -\sin \alpha \sin \theta \sin \Delta + \sin \alpha \cos \theta \cos \Delta \cos \phi + \sin \phi \cos \Delta \cos \alpha, \\
\sin \alpha \cos \theta \sin \phi - \cos \phi \cos \alpha, \\
-\sin \alpha \sin \theta \cos \Delta - \sin \alpha \cos \theta \cos \phi \sin \Delta - \sin \phi \sin \Delta \cos \alpha \rangle.
$$

Figure 3. The spontaneous polarization is along the direction given by the polarization director $\mathbf{p}$. 
This representation contains implicitly the constraints \(|n| = |p| = 1\) and \(n \cdot p = 0\), a fact which proves to be particularly useful when deriving bounds for the energy of specific states.

A popular reference book for the physics of LCs is [13] by de Gennes and Prost, while a mathematical introduction to classical results for nematic and smectic LCs are the books by Stewart [15], and Virga [17]. For an understanding of the properties and modeling of ferroelectric LCs standard references include Lagerwall [10] and Mušević & Blinc & Žekš [12].

3. Model. The Landau free energy density introduced in [16] includes some usual terms, that is the one-constant approximation Frank-Oseen nematic elastic energy, the Chen-Lubensky energy describing the smectic structure and the dipole-dipole self-interaction energy, as well as three terms pertinent to the bent-core molecules: a coupling term between the polarization splay and the tilt of the material molecules with respect to the normal vector of the smectic layers, a term proportional to the polarization splay and finally a coupling term between the polar and nematic parameters and the layer normal, which serves as penalization for deviation of the polarization from being parallel to \(n \times \nu\). Specifically, they propose the free energy density:

\[
\begin{align*}
\frac{1}{2} K_n \left[ (\nabla \cdot n)^2 + |\nabla \times n|^2 \right] + c_{||} |(n \cdot \nabla - i q_0) \psi|^2 + c_\perp |n \times \nabla \psi|^2 \\
+ D |(n \times \nabla)^2 \psi|^2 + \frac{P_0^2}{2\varepsilon \varepsilon_0} P_1^2 + k_p (\nabla \cdot p) |n \times \nabla \psi|^2 + \frac{1}{2} k_p (\nabla \cdot p)^2 \\
+ K_{np} |p \times (n \times \nabla \psi)|^2,
\end{align*}
\]

(2)

with the constraints \(|n| = |p| = 1\) and \(n \cdot p = 0\). Here, \(q_0 = \frac{2\pi}{d_0}\) where \(d_0\) is the smectic layer thickness in the non-tilted phase, \(P_1\) is the \(x\)-component of the polarization director, and all the coefficients are positive, except \(c_\perp\) which is taken to be strictly less than zero, as it is the case in the SmC phase. In postulating the form of the energy, the authors make the assumption that the problem of layer undulation formation starting from an homogenous tilted phase is essentially one-dimensional, therefore in the above expression everything depends only on the variable \(x\). The authors also assume that the polarization \(P = P_0 p\) has constant magnitude \(P_0\), and neglect the Maxwell’s equations in the electric self-interaction energy term, hence the simplified form of the self-interaction dipole term. An additional implicit assumption is that the material is well in the smectic phase so that \(|\psi|\) is constant.

The energy for bent-core molecules [3, 2012] and the one for ferroelectricity [4, 2013] used by Bauman and collaborators incorporate the full self-interaction energy term, but assume that the ground state of the system is the so-called SmC\(_G\) state, resulting in a different choice for the term describing the interaction between the polarization director, the layer normal and nematic director.

There are two mathematical shortcomings in the above energy. First, to show existence of energy minimizers it is well-known that the term involving the second order derivatives of the Chen-Lubensky smectic energy [6] needs to be modified, for example following the work of Luk’yanchuk [11], since in its original form does not allow for the control of the second derivatives of \(\psi\) in the \(n\) direction, [9]. Second, the quadratic term involving the divergence of \(p\) is not sufficient to mathematically control its gradient.
We use the Chen-Lubensky energy density introduced in [3], and consider the modifications mentioned above, so that the energy density in (2) becomes

\[
\begin{align*}
 f(\psi, \mathbf{n}, \mathbf{p}) &= \frac{1}{2} K_n \left[ |\nabla \cdot \mathbf{n}|^2 + |\nabla \times \mathbf{n}|^2 \right] + c_\parallel |D_{\parallel} \psi|^2 + c_\perp |D_{\perp} \psi|^2 \\
 &\quad + a_\parallel |D \cdot D_{\parallel} \psi|^2 + a_\parallel |D \cdot D_{\parallel} \psi|^2 + \frac{P_0^2}{2\epsilon_0} p_1^2 + \tilde{K}_p (\nabla \cdot \mathbf{p}) |D_{\perp} \psi|^2 \\
 &\quad + \frac{1}{2} K_p \left[ (\nabla \cdot \mathbf{p})^2 + |\nabla \times \mathbf{p}|^2 + K_n p \cdot ( \mathbf{n} \times D_{\perp} \psi) \right]^2,
\end{align*}
\]

(3)

where \( D_{\psi} = \nabla \psi - iq \cos \theta_B \mathbf{n} \psi \), and \( D_{\parallel}, D_{\perp} \) are its components parallel and perpendicular to the direction of the nematic vector, that is \( D_{\parallel} \psi = (\mathbf{n} \cdot \nabla \psi - i q \cos \theta_B \psi) \mathbf{n} \) and \( D_{\perp} \psi = D_{\psi} - D_{\parallel} \psi \). Here, \( q \) is the smectic layer periodicity along the \( z \)-axis, and \( q_0 = q \cos \theta_B \), with \( \theta_B \) the cone angle in the homogeneous phase.

The order parameter \( \psi \) describes the smectic layering, and corresponds to the distribution of the centers of mass of the molecules, more precisely:

\[
\psi(x, y, z) = \eta(x, y, z)e^{i\omega(x, y, z)},
\]

where \( \eta_0 + \eta(x, y, z) \cos(\omega(x, y, z)) \) is the molecular mass density, \( \eta_0 \) the locally uniform mass density and \( \eta \) the mass density of the smectic layers. The smectic layers themselves are the level sets of \( \omega \). Therefore, if \( \psi = 0 \) the molecules have no positional order, the centers of masses are distributed uniformly, and the liquid crystal is in the nematic phase. The assumption that the phenomenon under investigation is essentially one-dimensional is reflected in the choice the authors make for \( \psi \) in [16], they consider \( \eta(x, y, z) = \eta \) constant and \( \omega(x, y, z) = q(z + u(x)) \), where \( u(x) \) measures the displacement from the unmodulated structure. Rewriting the energy in terms of \( u \), and the components of \( \mathbf{n}(x) = (n_1(x), n_2(x), n_3(x)) \) and \( \mathbf{p}(x) = (p_1(x), p_2(x), p_3(x)) \) yields:

\[
\begin{align*}
 f(u, \mathbf{n}, \mathbf{p}) &= \frac{1}{2} K_n \left[ (n_1')^2 + (n_2')^2 + (n_3')^2 \right] + c_\parallel \eta^2 q^2 (u' n_1 + n_3 - \cos \theta_B)^2 \\
 &\quad - |c_\perp| \eta^2 q^2 \left[ (u')^2 - 1 - (u' n_1 + n_3)^2 \right] + a_\perp \eta^2 q^2 \left[ (u')^2 - 1 - (u' n_1 + n_3)^2 \right]^2 \\
 &\quad + a_\perp \eta^2 q^2 \left[ (u' - (u' n_1 + n_3)) n_1 \right]^2 + a_\parallel \eta^2 q^2 \left[ (u' n_1 + n_3 - \cos \theta_B)^4 \\
 &\quad + a_\parallel \eta^2 q^2 \left[ (u' n_1 + n_3 - n_1 \cos \theta_B)^2 \right]^2 + \frac{P_0^2}{2\epsilon_0} p_1^2 \\
 &\quad + \tilde{K}_p \eta^2 q^2 \left[ (u')^2 - 1 - (u' n_1 + n_3)^2 \right] p_1^2 + \frac{1}{2} K_p \left[ (p'_1)^2 + (p'_2)^2 + (p'_3)^2 \right] \\
 &\quad + K_{np} \eta^2 q^2 (u' p_1 + p_3)^2.
\end{align*}
\]

(4)

For a fixed bounded interval \( \Omega = (a, b) \), we let

\[
\mathcal{A} = \{ (u, \mathbf{n}, \mathbf{p}) : u \in H^2(\Omega), \mathbf{n}, \mathbf{p} \in H^1(\Omega; S^2) \text{ with } \mathbf{n} \cdot \mathbf{p} = 0 \text{ in } \Omega \},
\]

and define the free energy:

\[
\mathcal{F}(u, \mathbf{n}, \mathbf{p}) = \int_\Omega f(u, \mathbf{n}, \mathbf{p}) \, dx.
\]

**Proposition 1.** The functional \( \mathcal{F} \) is bounded below in the class of functions \( (u, \mathbf{n}, \mathbf{p}) \in \mathcal{A} \),

which verifies either periodic boundary conditions for \( u', n_1 \) and \( p_1 \), or zero boundary conditions only for \( p_1 \). More precisely, for such functions there are positive constants
For any $\epsilon > 0$, and real numbers $c$ and $d$, we have for fixed $\epsilon_0, \epsilon_1 > 0$:

$$a_\perp [(u')^2 + (u' n_1 + n_3) n_1']^2 + a\parallel [(u' n_1 + n_3) n_1 - n_1 \cos \theta_B)]^2$$

$$\geq \min \left\{ a_\perp, a\parallel \right\} \left[ \frac{\epsilon_0}{1+\epsilon_0} (u'')^2 + \left( \frac{\epsilon_1}{1+\epsilon_1} - \epsilon_0 \right) [(u' n_1 + n_3) n_1']^2 + \epsilon_1 \cos^2 \theta_B (n'_1)^2 \right]$$,

as well as, for fixed $\epsilon_2 > 0$:

$$a_\perp [(u')^2 + 1 - (u' n_1 + n_3)]^2 \geq a_\perp \frac{\epsilon_2}{1+\epsilon_2} [(u')^2 + 1]^2 - a_\perp \epsilon_2 (u' n_1 + n_3)^4.$$
Recalling that $|\eta| = 1$, and using (7) and (8) in equation (6), leads to our next inequality:

$$
\mathcal{F}(u, n, p) \geq \int_\Omega \left[ \left( \frac{K_n}{2} - \frac{\epsilon_7}{\epsilon_9} \int_\Omega (u'')^2 dx - \frac{1}{\epsilon_{10}} \int_\Omega (u'')^2 n_1^2 p_1^2 dx \right) \right] dx. \quad (7)
$$

with

$$
\int_\Omega (u'')^2 dx - \frac{1}{\epsilon_{10}} \int_\Omega (u'')^2 n_1^2 p_1^2 dx \geq -\epsilon_{11} \int_\Omega (u'')^2 dx. \quad (8)
$$

Recalling that $|p| = |n| = 1$, and using (7) and (8) in equation (6), leads to our next inequality:

$$
\mathcal{F}(u, n, p) \geq \int_\Omega \left[ \left( \frac{K_n}{2} - \frac{\epsilon_7}{\epsilon_9} \int_\Omega (u'')^2 dx - \frac{1}{\epsilon_{10}} \int_\Omega (u'')^2 n_1^2 p_1^2 dx \right) \right] dx. \quad (7)
$$

with

$$
\int_\Omega (u'')^2 dx - \frac{1}{\epsilon_{10}} \int_\Omega (u'')^2 n_1^2 p_1^2 dx \geq -\epsilon_{11} \int_\Omega (u'')^2 dx. \quad (8)
$$
which is verified for any $\epsilon_j > 0$, $j = 1, 2$ and $j = 5..11$.

To obtain the wanted lower bound, we start by choosing $\epsilon_1$ small enough to have $K_p - \frac{1}{2} \min \{a_\perp, a_\parallel\} \eta^2 q_2 \epsilon_1 \cos \theta_B > C_0 > 0$ for some constant $C_0$; then we select $\epsilon_5, \epsilon_7$ and $\epsilon_{10}$ so to have the coefficient of the $(u'')^2$ term positive, say greater of a constant $C_1 > 0$, and after that we pick $\epsilon_6$ small enough to verify $C_0 - a_\perp \eta^2 q_2 \epsilon_5 \epsilon_6 > C_2 > 0$, for some constant $C_2$. Once, $\epsilon_5$ and $\epsilon_6$ are fixed, we can find an $\epsilon_{11}$ for which the coefficient of $(u' n_1 n'_1)^2$ is a positive constant, denoted by $C_3$. Finally, we choose $\epsilon_8$ and $\epsilon_9$ so that the coefficient of $|p'|^2$ is greater than some constant $C_4 > 0$, and $\epsilon_2$ so that the one of $(u' n_1 + n_3)^4$ is greater than some constant $C_5 > 0$.

If we next set $C_0 = K_p \eta^2 q_2 \left( \frac{1}{\epsilon_7} + \frac{1}{\epsilon_8} + \frac{1}{\epsilon_{10}} + \frac{1}{\epsilon_{11}} \right)$, $C_7 = \frac{K_p \eta^2 q_2}{\epsilon_9} |\Omega|$, and $C_8 = \frac{a_\perp \epsilon_2}{2} - \eta^2 q_4^4$, we are left with the inequality:

$$
\mathcal{F}(u, \mathbf{n}, \mathbf{p}) \geq \int_{\Omega} \left[ C_2 \left( n_1'^2 + (n_2')^2 + (n_3')^2 \right) + a_\parallel \eta^2 q_2 (u' n_1 + n_3 - \cos \theta_B)^2 - |c_\perp| \eta^2 q_2 \left( (u')^2 + 1 - (u' n_1 + n_3)^2 \right) \right. \\
+\frac{a_\parallel \epsilon_7}{2} \eta^2 q_4 \left( (u')^2 + 1 - (u' n_1 + n_3)^2 \right)^2 + \frac{a_\parallel}{2} \eta^2 q_4 (u' n_1 + n_3 - \cos \theta_B)^4 \\
+C_8 \left( (u')^2 + 1 \right)^2 + C_5 (u' n_1 + n_3)^4 \\
-\frac{a_\parallel}{4} \eta^2 q_4 \cos^2 \theta_B (u' n_1 + n_3)^2 - \frac{a_\parallel}{2} \eta^2 q_4 \cos^2 \theta_B (u' n_1 + n_3 - \cos \theta_B)^2 \\
+\frac{a_\parallel}{2} \eta^2 q_4 \left( (u' n_1 + n_3) n_1 - n_1 \cos \theta_B \right)^2 \\
+C_3 (u' n_1 n'_1)^2 + C_1 (u' n_1)^2 + C_5 (u')^2 + C_4 \left[ (p'_1)^2 + (p'_2)^2 + (p'_3)^2 \right] \\
+\frac{P_0^2}{2 \epsilon_6} p_1^2 + K_{np} \eta^2 q_2 (u' p_1 + p_3)^2 \right] \, dx - C_7, 
$$

for some positive constants $C_j > 0$, $j = 1..8$.

We let $C = \min\{C_1, C_2, C_4, 2 C_8\}$, and use in (10) the elementary bound $\alpha t^2 - \beta t \geq -\frac{\beta^2}{2\alpha}$, which holds for every $\alpha, \beta > 0$, to conclude that there exist positive
constants \( C \) and \( \tilde{C} \) such that
\[
F(u, n, p) \geq K_{np} \eta^2 q^2 \int_{\Omega} (u^p_1 + p_3)^2 \, dx \\
+ C \int_{\Omega} [(u'')^2 + (u')^2 + |n|^2 + |p'|^2] \, dx - \tilde{C},
\]
and the proposition follows. \( \square \)

The previous proposition implies the existence of minimizers of \( F \) in the following classes of functions:
\[
A_0 = \left\{ (u, n, p) \in A \text{ with } u \big|_{\partial \Omega} = p_1 \big|_{\partial \Omega} = 0 \right\},
\]
\[
A_p = \left\{ (u, n, p) \in A \text{ with periodic boundary conditions for } u', n_1 \text{ and } p_1 \right\}.
\]

**Proposition 2.** There exist minimizers for \( F \) in \( A_0 \) and \( A_p \).

**Proof.** We will first prove the result for \( A_0 \), and then point out the modifications needed for the proof with \( A_p \). The energy functional \( F \) is bounded below, by Proposition 1, and above, since if we pick \( n_0 = (1, 0, 0) \) and \( p_0 = (0, 1, 0) \) we have that \( F(0, n_0, p_0) = \eta^2 q^2 |\Omega| \left[c_0 \cos^2 \theta_B - |c_1| + a_1 q^2 + a_2 q^2 \cos \theta_B \right] \).

Therefore, we can consider a minimizing sequence \( \{(u_j, n_j, p_j)\} \subset A_0 \), namely \( F(u_j, n_j, p_j) \to \inf_{(u, n, p) \in A_0} F(u, n, p) \), and from (5) for any \( c > 0 \) fixed, we can find a \( j_c \) such that
\[
C \int_{\Omega} [(u''_j)^2 + (u'_j)^2 + |n_j|^2 + |p_j'|^2] \, dx - \tilde{C} \\
\leq F(u_j, n_j, p_j) \leq \inf_{(u, n, p) \in A_0} F(u, n, p) + c,
\]
for any \( j > j_c \). From this inequality, since \( \|n_j\|_{L^2(\Omega)} = \|p_j\|_{L^2(\Omega)} = |\Omega|^{1/2} \), and due to the zero boundary conditions on \( u_j \), we conclude that \( \{(u_j, n_j, p_j)\} \) is uniformly bounded in \( H^2(\Omega) \times H^1(\Omega; \mathbb{R}^3) \times H^1(\Omega; \mathbb{R}^3), \forall j > j_c \). Hence, there exists a subsequence, still denoted by \( (u_j, n_j, p_j) \), such that \( (u_j, n_j, p_j) \rightharpoonup (u_{\infty}, n_{\infty}, p_{\infty}) \) weakly in \( H^2(\Omega) \times H^1(\Omega; \mathbb{R}^3) \times H^1(\Omega; \mathbb{R}^3) \), see [5, Theorem 3.18], strongly in \( H^1(\Omega) \times L^2(\Omega; \mathbb{R}^3) \times L^2(\Omega; \mathbb{R}^3) \), by the Rellich-Kondrachov Compactness Theorem [1], and such that \( u_j, u'_j, n_j, p_j \) all converge almost everywhere in \( \Omega \), [1, pg 30]. In fact, since \( \Omega \subset \mathbb{R} \) and bounded, we know that \( H^{j+1}(\Omega) \subset C^{j, \lambda}(\Omega) \) for \( j = 0, 1 \) and \( 0 < \lambda < \frac{1}{2} \) always compact imbedding, so the convergence is uniform, [1, pg 168]. From this, it is straightforward to conclude that \( (u_{\infty}, n_{\infty}, p_{\infty}) \in A_0 \). By the weak lower semicontinuity of the \( L^2 \) norm, and Proposition 3.5 in [5], since \( [(u'_j)^2 + 1 - (u'_j (n_j)_1 + (n_j)_3)^2] \) converges strongly in \( L^2 \), we have
\[
F(u_{\infty}, n_{\infty}, p_{\infty}) \leq \liminf_{j \to \infty} F(u_j, n_j, p_j) = \inf_{(u, n, p) \in A_0} F(u, n, p).
\]

For functions in \( A_p \), the lower and upper bounds on the energy, which are still valid, allows us to find as before a subsequence whose nematic and polarization directors converge to suitable \( n_{\infty} \) and \( p_{\infty} \). Instead, for the \( u_j \)'s we can assume that the subsequence \( u'_j \) converges weakly in \( H^1(\Omega) \), strongly in \( L^2(\Omega) \) and uniformly to a function \( w_{\infty} \in H^1(\Omega) \), such that \( w_{\infty}(0) = w_{\infty}(1) \), this last condition due to the periodic boundary conditions on the \( u'_j \) and the uniform convergence in \( \Omega \). Hence, the function \( u_{\infty}(x) = \int_0^x w_{\infty}(t) \, dt \) is such that \( (u_{\infty}, n_{\infty}, p_{\infty}) \in A_p \). The proposition then follows if we notice that \( w_j(x) = u_j(x) - u_j(0) \) converges weakly
in $H^2(\Omega)$, strongly in $H^1(\Omega)$ and uniformly to $u_\infty$, and verifies $\mathcal{F}(w_j, n_j, p_j) = \mathcal{F}(u_j, n_j, p_j)$.

4. Columnar phases simplified model.

4.1. Model and notations. The so-called $B_1$ phase observed in bent-core molecule liquid crystals is characterized by a two-dimensional structure, where columns of broken smectic layers result in an antiferroelectric structure. In this phase the spontaneous polarization is perpendicular to the column axis, if instead the polarization is along the column axis, the material is in a so-called reversed $B_1$ phase, denoted by $B_{1\text{rev}}$ or $B_{1\text{rev tilted}}$, depending if the nematic director is parallel or tilted with respect to the normal of the smectic layers, [7, 8]. The experimental work presented in [8] deals with both reversed $B_1$ phases, since in these phases the spontaneous polarization can be reoriented using an electric field, without a complete rebuilding of the underlining columnar structure. The modeling and numerical part is dedicated to the study of the $B_{1\text{rev tilted}}$ phase, where the tilt allows the molecules to switch polarization either by rotating around the molecular axis or around the cone, or more in general by a combination of both, see Figure 4.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{Schematic representation of the $B_{1\text{rev tilted}}$ phase structure, and switching by an external electric field}
\end{figure}

In particular, the authors are interested in the dependence on physical parameters of the type of switching, that is in knowing if the rotation is along the axis of the molecules or the cone for particular materials and sample size, since the two different rotations have different consequences on the structural chirality. They adopt an energy, inspired by the density (2), which includes a term that accounts for the interaction of the external electric field $E$ and the polarization. They observe that in the $B_{1\text{rev tilted}}$ phase normal and the tilt angle $\theta$ are constant, so that $\theta = \theta_B \neq 0$ or $\pi$, and all the terms involving only the smectic order parameter are
constant. In here, to represent this situation, we consider the energy density:

\[
\frac{1}{2} K_n \left[ (\nabla \cdot \mathbf{n})^2 + |\nabla \times \mathbf{n}|^2 \right] + \frac{P_0^2}{2\varepsilon_0} p_1^2 + \hat{K}_p (\nabla \cdot \mathbf{p}) |\mathbf{n} \times \mathbf{\nu}|^2 + \frac{1}{2} K_p \left[ (\nabla \cdot \mathbf{p})^2 + |\nabla \times \mathbf{p}|^2 \right] + \hat{K}_{np} |\mathbf{p} \times (\mathbf{n} \times \mathbf{\nu})|^2 - P_0 \mathbf{p} \cdot \mathbf{E},
\]

where \( \mathbf{\nu} \) is the layer normal.

We non-dimensionalize the energy by rescaling distances with respect to the column width \( L \), and multiply it by the factor \( \frac{2\varepsilon_0}{P_0^2} \). As in [8], we also consider a reference frame with the \( y \)-axis parallel to the columnar axis, so that \( \mathbf{\nu} = \mathbf{e}_3 \equiv <0, 0, 1> \), and take the applied electric field in the same direction as the columnar axis, that is \( \mathbf{E} = E \mathbf{e}_2 \). In conclusion, using the fact that \( |\mathbf{n} \times \mathbf{\nu}|^2 = \sin^2 \theta_B \), we are lead to work with the following non-dimensionalized energy functional:

\[
\mathcal{E}_L(\mathbf{n}, \mathbf{p}) = \int_D e_L(\mathbf{n}, \mathbf{p}) \, dx,
\]

where \( D = (0, 1) \), and

\[
e_L(\mathbf{n}, \mathbf{p}) = \frac{1}{2} \frac{K_n}{L} \left[ (n_1')^2 + (n_2')^2 + (n_3')^2 \right] + \frac{1}{2} \frac{K_p}{L} \left[ (p_1')^2 + (p_2')^2 + (p_3')^2 \right] + L p_1^2 + \hat{k}_p^* \sin^2 \theta_B p_1' + \frac{1}{2} L k_{np} p_3^2 + \frac{1}{2} L |k_E| \left[ p_1^2 + (p_2 - \text{sgn}(E))^2 + p_3^2 \right],
\]

with

\[
k_n^* = \frac{2\varepsilon_0}{P_0^2} K_n; \quad \hat{k}_p^* = \frac{2\varepsilon_0}{P_0^2} \hat{K}_p; \quad k_p^* = \frac{2\varepsilon_0}{P_0^2} K_p; \quad k_{np} = 2\hat{K}_{np} \frac{2\varepsilon_0}{P_0^2}; \quad k_E = \frac{2\varepsilon_0}{P_0^2} E.
\]

To mimic the switching mechanism, we consider the boundary conditions:

\[
\mathbf{p}(0) = \mathbf{p}(1) = <0, -1, 0> \quad \text{and} \quad \mathbf{n}(0) = \mathbf{n}(1) = <\sin \theta_B, 0, \cos \theta_B>,
\]

and take \( E > 0 \) so that the applied electric field is in the opposite direction as the spontaneous polarization at the boundary.

This boundary conditions reflect the observation made in [8] that in a sample only the molecules of every other column will rotate, which can be modeled by considering only one single column with strong anchoring of the directors at the boundary. In particular, this implies the use of zero boundary conditions for the first component of the polarization director \( \mathbf{p} \).

Under these assumptions the energy can be written as:

\[
\mathcal{E}_L(\mathbf{n}, \mathbf{p}) = \int_D \left[ \frac{1}{2} \frac{k_n^*}{L} \left[ (n_1')^2 + (n_2')^2 + (n_3')^2 \right] + \frac{1}{2} \frac{k_p^*}{L} \left[ (p_1')^2 + (p_2')^2 + (p_3')^2 \right] + L p_1^2 + \frac{1}{2} L k_{np} p_3^2 + \frac{1}{2} L |k_E| \left[ p_1^2 + (p_2 - 1)^2 + p_3^2 \right] \right] \, dx.
\]

In what follows, we study how the relative size of the physical parameters in the energy density influence the minimizing states in the case of large column width. More precisely, we consider the \( \Gamma \)-limit of the energy for \( L \) tending to infinity, and study the minimizers of the limiting energy.
Remark 1. While considering the limiting behavior as the width of the column tends to infinity is consistent with the discussion in [8], one could take the point of view of keeping the width fixed, and let the elasticity constants become small relatively to the electric and coupling constants. In this interpretation, one could still work with the family of energies (16), where now $L^1$ would be the mathematical parameter expressing the relative behavior of the different constants. A mathematical analysis similar to the one below could then be applied.

We recall that given a metric space $X$ and a family of functionals $F_L : X \to [-\infty, \infty]$, parameterized by $L$, we say that $F_L \Gamma$-converges to a functional $F_\infty : X \to [-\infty, \infty]$ on $X$ as $L \to \infty$ if the following two conditions are satisfied:

(i) Liminf inequality: For every $x \in X$, and every sequence $\{x_L\} \subset X$ converging to $x$, we have
\[
\liminf_{L \to \infty} F_L(x_L) \geq F_\infty(x).
\]

(ii) Limsup inequality: For every $x \in X$, there exists a sequence $\{x_L\} \subset X$ converging to $x$ for which
\[
\limsup_{L \to \infty} F_L(x_L) \leq F_\infty(x).
\]

In this paper, to study the behavior of the energy minimizers for the large domain case, we consider the space:
\[
X = \{ (n, p) : \overline{D} \to S^2 \text{ measurable functions, with } n \cdot p = 0, \\
n_3 = \cos \theta_B, \ n(0) = n(1) = \langle \sin \theta_B, 0, \cos \theta_B \rangle, \\
p(0) = p(1) = (-0, -1, 0) \}. \]

As expected, the minimizers of the limiting energy, obtained considering the $L^1$ metric, belong to the the following subspace of $X$:
\[
Y_2 = \{ (n, p) \in Y \text{ such that } S(p_2) = 2 \} \subset X,
\]
where $S(v)$ = number of points of discontinuity of $v$, and
\[
Y = \{ (n, p) \text{ such that } p_2 \in BV_l(D; \{-1, 1\}), \quad p_2 = 1 \text{ in } D, \\
n_1 \in BV_r(D; \{-\sin \theta_B, \sin \theta_B\}), \quad n_3 = \cos \theta_B, \quad p_1 = p_3 = n_2 = 0 \},
\]
with
\[
BV_l(D; \{-1, 1\}) = \{ v \in BV(0, 1) \text{ with values in } \{-1, 1\}, \\
\text{and such that } v(0) = v(1) = -1 \}.
\]

We recall that functions in $BV(0, 1)$ are continuous, with possibly a finite number of jump discontinuities. Thus, in the above, if $x = 0$ or $x = 1$ are points of discontinuity of $v$, the boundary conditions are intended as $v(0^-) = v(1^+) = -1$, in other words, $BV_l(D; \{-1, 1\})$ can be identified with the space of functions $v \in BV_{loc}(\mathbb{R})$ with values in $\{-1, 1\}$, such that $v \equiv -1$ on $(-\infty, 0) \cup (1, \infty)$, [14]. The space $BV_r(D; \{-\sin \theta_B, \sin \theta_B\})$ is defined in an analogous way, with now boundary conditions $v(0) = v(1) = \sin \theta_B$. 
The expression of the limiting energy for functions \((\mathbf{n}, \mathbf{p}) \in Y_2\) is given by:

\[
\mathcal{F}(\mathbf{n}, \mathbf{p}) = \inf_{T \geq 0} \inf \left\{ (N - 2) \int_T^{T} E(\mathbf{w}, \mathbf{z}) \, dx \right\} + \inf_{T \geq 0} \left\{ \int_{-T}^{T} E(\mathbf{v}, \mathbf{u}) \, dx \right\}
\]

\[+ \inf_{T \geq 0} \left\{ \int_{-T}^{T} E(\mathbf{v}_1, \mathbf{u}_1) \, dx \right\},\]

where \(N\) is the total number of points of discontinuity of \(n_1\) and \(p_2\) counted once, and the first infimum is taken over functions \(\mathbf{w}, \mathbf{z}, \mathbf{v}, \mathbf{u}, \mathbf{v}_1, \mathbf{u}_1 \in H^1((-T, T); S^2)\), such that

\[
\mathbf{w}(\pm T) = (\pm \sin \theta_B, 0, \cos \theta_B); \quad \mathbf{v}(\pm T) = (n_1(0^\pm), 0, \cos \theta_B);
\]

\[
\mathbf{v}_1(\pm T) = (n_1(1^\pm), 0, \cos \theta_B);
\]

\[
\mathbf{z}(\pm T) = (0, 1, 0); \quad \mathbf{u}(\pm T) = (0, \pm 1, 0); \quad \mathbf{u}_1(\pm T) = (0, \mp 1, 0);
\]

\[
\mathbf{w} \cdot \mathbf{z} = 0; \quad \mathbf{v} \cdot \mathbf{u} = 0; \quad \mathbf{v}_1 \cdot \mathbf{u}_1 = 0;
\]

\[
w_3 = \cos \theta_B; \quad v_3 = \cos \theta_B; \quad (v_1)_3 = \cos \theta_B;
\]

and

\[
E(\mathbf{a}, \mathbf{b}) = \frac{1}{2} \left( k_n^* |a'|^2 + k_p^* |b'|^2 \right) + b_1^2 + \frac{1}{2} k_{np} b_2^2 + \frac{1}{2} |k_E| \left[ b_1^2 + (b_2 - 1)^2 + b_3^2 \right].
\]

Finally, we extend the energy functional in a standard fashion so that it will be defined for all functions in \(X\):

\[
\mathcal{F}_L(\mathbf{n}, \mathbf{p}) = \begin{cases} 
E_L(\mathbf{n}, \mathbf{p}) & \text{if } (\mathbf{n}, \mathbf{p}) \in (H^1(D; S^2) \times H^1(D; S^2)) \cap X \\
\infty & \text{if } (\mathbf{n}, \mathbf{p}) \in X \setminus (H^1(D; S^2) \times H^1(D; S^2)),
\end{cases}
\]

and similarly for the limiting functional:

\[
\mathcal{F}_\infty(\mathbf{n}, \mathbf{p}) = \begin{cases} 
\mathcal{F}(\mathbf{n}, \mathbf{p}) & \text{if } (\mathbf{n}, \mathbf{p}) \in Y_2 \\
\infty & \text{if } (\mathbf{n}, \mathbf{p}) \in X \setminus Y_2.
\end{cases}
\]

### 4.2. Compactness and \(\Gamma\)-convergence

We start by deriving a compactness result.

**Proposition 3 (Compactness).** Let \(L_k \to \infty\) and \(\{(\mathbf{n}_k, \mathbf{p}_k)\} \subset X\) such that \(\mathcal{F}_{L_k}(\mathbf{n}_k, \mathbf{p}_k)\) is uniformly bounded, then \(\{(\mathbf{n}_k, \mathbf{p}_k)\}\) is pre-compact in \(X\), that is there exists \((\mathbf{n}, \mathbf{p}) \in Y_2 \subset X\) and a subsequence \(\{(\mathbf{n}_{k_j}, \mathbf{p}_{k_j})\}\) such that \((\mathbf{n}_{k_j}, \mathbf{p}_{k_j}) \to (\mathbf{n}, \mathbf{p})\) in the \(L^1\)-norm.

**Proof.** Assume there exists \(M > 0\) independent of \(k\) such that

\[
0 \leq \mathcal{F}_{L_k}(\mathbf{n}_k, \mathbf{p}_k) \leq M,
\]

then by definition of \(\mathcal{F}_{L_k}\) we deduce that \((\mathbf{n}_k, \mathbf{p}_k) \in H^1(D; S^2) \times H^1(D; S^2)\).

Additionally, if we denote by \((p_{1k})_k\) and \((n_{jk})_k, j = 1, 2, 3\), the components of the vectors \(\mathbf{p}_k\) and \(\mathbf{n}_k\), we see that

\[
\int_0^1 (p_{1k})^2 \, dx \leq \frac{M}{L_k}, \quad \int_0^1 (p_{3k})^2 \, dx \leq \frac{2M}{L_k k_{np}}, \quad \int_0^1 [(p_{2k}) - 1]^2 \, dx \leq \frac{2M}{L_k |k_E|},
\]

hence, as \(L_k \to \infty\), we have \((p_{1k})_k \to 0, (p_{2k})_k \to 1\) and \((p_{3k})_k \to 0\) in \(L^2(D)\), and \(D\) bounded implies that they also converge in \(L^1(D)\) and a.e. up to subsequences.
Looking at boundary condition, since \( (p_2)_k \) has a continuous representative, we can extend it to the whole real line as follows:

\[
(\tilde{p}_2)_k = \begin{cases} 
(p_2)_k, & \text{if } x \in D \\
-1, & \text{if } x \in \mathbb{R} \setminus D,
\end{cases}
\]

so that \( (\tilde{p}_2)_k \in L^1_{\text{loc}}(\mathbb{R}) \), and

\[
(\tilde{p}_2)_k \to \begin{cases} 
1, & \text{if } x \in D \\
-1, & \text{if } x \in \mathbb{R} \setminus D,
\end{cases}
\]

pointwise a.e. up to subsequences, and in \( L^1_{\text{loc}}(\mathbb{R}) \). In other words, \( (p_2)_k \to p_2 \in BV(\mathbb{R}; \{-1, 1\}) \) in the \( L^1 \)-norm.

Again from the uniform bound for the energies of the elements of the sequence, since

\[
(p_3)_k^2 = |p_k \times (n_k \times \nu)|^2 = (n_1^2 + n_2^2) - (n_1 p_2 - n_2 p_1)^2,
\]

we have, where we drop the subscript \( k \) for simplicity of notation, that

\[
M \geq \frac{1}{2} L_{kp} \int_0^1 \left[ (n_1^2 + n_2^2) - (n_1 p_2 - n_2 p_1)^2 \right] dx
\]

\[
= \frac{1}{2} L_{kp} \int_0^1 \left( \sin^2 \theta_B - n_1^2 p_2^2 - n_2^2 p_1^2 + 2 n_1 p_1 n_2 p_2 \right) dx
\]

\[
= \frac{1}{2} L_{kp} \int_0^1 \left[ (\sin^2 \theta_B - n_1^2) + n_1^2 (1 - p_2^2) - n_2^2 p_1^2 + 2 n_1 p_1 n_2 p_2 \right] dx
\]

\[
= \frac{1}{2} L_{kp} \int_0^1 \left[ (\sin^2 \theta_B - n_1^2) + n_1^2 (1 - p_2^2) - n_2^2 p_1^2 + 2 n_1 p_1 n_2 p_2 \right] dx
\]

\[
= \frac{1}{2} L_{kp} \int_0^1 \left[ (\sin^2 \theta_B - n_1^2) + n_1^2 (1 - p_2^2) - n_2^2 p_1^2 + 2 n_1 p_1 n_2 p_2 \right] dx
\]

\[
\leq M + \frac{1}{2} L_{kp} \int_0^1 n_2^2 p_1^2 dx + \frac{1}{2} L_{kp} \int_0^1 2 n_2^2 p_1^2 dx + \frac{1}{2} L_{kp} \int_0^1 2 n_3 p_3 n_1 p_1 dx
\]

\[
\leq M + \frac{1}{2} L_{kp} \int_0^1 p_1^2 dx + \frac{1}{2} L_{kp} \int_0^1 \left( 3 n_1^2 p_1^2 + n_3^2 p_3^2 \right) dx
\]
\[ \leq M + \frac{1}{2} k_{np} \left( L \int_0^1 p_1^2 dx \right) + \frac{3}{2} k_{np} \left( L \int_0^1 p_1^2 dx \right) + \frac{1}{2} L k_{np} \int_0^1 p_2^2 dx \]
\[ \leq 2 k_{np} M + 2 M. \]  

Equation (20) allows us to follow the classical Modica-Mortola argument for the term involving \( n_1 \). Namely, we start by noticing that

\[ \sqrt{k_{np} k_n^*} \int_0^1 \sqrt{\sin^2 \theta_B - n_1^2} |n_1'| dx \leq \frac{1}{2} L k_{np} \int_0^1 (\sin^2 \theta_B - n_1^2) dx \]
\[ + \frac{1}{2} k_n^* \int_0^1 (n_1')^2 dx \leq 2M + 2 k_{np} M + M, \]  

then we define \( \phi_1(t) = \int_{-\sin \theta_B}^{t} \sqrt{\sin^2 \theta_B - s^2} ds \), so that the change of variable \( t = n_1(x) \), and the chain rule in \( W^{1,1}(D) \), here \( \phi_1 \in C^1([-\sin \theta_B, \sin \theta_B]) \), give

\[ 3M + 2 k_{np} M \geq \sqrt{k_{np} k_n^*} \int_0^1 \sqrt{\sin^2 \theta_B - n_1^2(x)} |n_1'(x)| dx \]
\[ = \sqrt{k_{np} k_n^*} \int_0^1 |(\phi_1(n_1(x)))'| dx, \]

that is, \( [\phi_1(n_1(x))]' \) is uniformly bounded in \( L^1(D) \). On the other hand, since \( |n_1(x)| \leq \sin \theta_B \), we have \( |\phi_1(n_1(x))| \leq 2 \sin^2 \theta_B \), which implies \( \phi_1(n_1(x)) \) is uniformly bounded in \( L^1(D) \). In conclusion, reintroducing the subscript \( k \), the sequence of functions \( W_k := \phi_1 \circ (n_{1k}) \) is uniformly bounded in \( W^{1,1}(D) \).

By the Rellich–Kondrachov theorem, there exists a subsequence of \( \{(n_{1k})\} \), which we still label with \( k \), and a function \( W \in BV(D) \) such that \( W_k := \phi_1 \circ (n_{1k}) \rightarrow W \) in \( L^1_{loc}(D) \), also by taking a further subsequence, we can assume \( W_k(x) \rightarrow W(x) \) a.e. in \( D \).

From (20), the function \( w((n_{1k})(x)) = \sin^2 \theta_B - (n_{1k})^2(x) \) is such that

\[ \int_0^1 |w((n_{1k})(x))| dx = \int_0^1 (\sin^2 \theta_B - (n_{1k})^2(x)) dx \leq \frac{4}{L_k} \left( \frac{M}{k_{np}} + M \right), \]  

and, for \( L_k \rightarrow \infty \) we have \( w((n_{1k})) \rightarrow 0 \) in \( L^1(D) \), a.e. up to a subsequence.

\( \phi_1(t) \) is continuous and strictly increasing in \( [-\sin \theta_B, \sin \theta_B] \), hence \( \phi_1^{-1} \) is continuous and \( (n_{1k})(x) = \phi_1^{-1}(W_k(x)) \rightarrow \phi_1^{-1}(W(x)) \) a.e. We set \( n_1(x) := \phi_1^{-1}(W(x)) \), and remark that since \( w((n_{1k})(x)) \rightarrow 0 \) a.e. in \( D \) it must hold \( w(n_1(x)) = 0 \) a.e. in \( D \), which gives \( n_1(x) \in \{-\sin \theta_B, \sin \theta_B\} \) a.e. in \( D \).

In turn, \( W(x) \in \{\phi_1(-\sin \theta_B), \phi_1(\sin \theta_B)\} \), but \( \phi_1(-\sin \theta_B) = 0 \), so there exists a set \( E \subset D \) such that \( W(x) = \phi_1(\sin \theta_B) \chi_E \). Now, \( W \in BV(D) \) and \( D \) has finite measure thus \( \chi_E \in BV(D) \), and \( n_1 = \sin \theta_B \chi_E - \sin \theta_B (1 - \chi_E) \). From this, we conclude that \( (n_{1k}) \) converges a.e. in \( D \) to a BV function with values in \( \{-\sin \theta_B, \sin \theta_B\} \). Furthermore, if outside \( D \) we extend \( (n_{1k}) \) to be \( \sin \theta_B \), we
obtain that \((n_1)_k \to \sin \theta_B\) a.e. in \((\mathbb{R} \setminus D)\), we can then conclude that \((n_1)_k\) converges a.e. to a \(BV_r(D; \{\sin \theta_B, \sin \theta_B\})\) function.

Convergence of \((n_1)_k\) in \(L^1(\mathbb{R})\) follows by Egoroff’s and Vitali’s convergence theorems if we show \(\{n_k\}\) is equi-integrable, i.e. for all \(\varepsilon > 0\) there exists \(\delta > 0\) such that \(\int |n_k| d\mu \leq \varepsilon\) for all \(k\) and \(F \subset D\) with \(\mu(F) \leq \delta\), but since \(|n_k| = 1\), \(\int_F |n_k| d\mu \leq \mu(F)\), we can pick \(\delta = \varepsilon\).

Finally, using the fact that \((n_1)^2_k + (n_2)^2_k = \sin^2 \theta_B\) we also have that \((n_2)_k\) converges to 0 in \(L^1\) and a.e. \(\square\)

We are able to prove the following standard \(\Gamma\)-convergence result:

**Theorem 4.1.** Consider \(X\) as a metric space endowed with the \(L^1\)-norm, then for \(L \to \infty\) the functional \(F_L\) \(\Gamma\)-converges to \(F_\infty\).

**Proof.** **Limsup Inequality:** Consider \((n, p) \in X\) and \(\{n_k, p_k\} \subset X\) such that \((n_k, p_k) \to (n, p)\) in \(L^1\), we need to show that

\[
\lim_{L_k \to \infty} \inf \mathcal{F}_{L_k}(n_k, p_k) \geq \mathcal{F}_\infty(n, p).
\]

If \(\lim_{L_k \to \infty} \inf \mathcal{F}_{L_k}(n_k, p_k) = \infty\) there is nothing to prove, otherwise there exists a subsequence such that \(\lim_{j \to \infty} \mathcal{F}_{L_{k_j}}(n_{k_j}, p_{k_j}) = \lim_{j \to \infty} \inf \mathcal{F}_{L_{k_j}}(n_{k_j}, p_{k_j}) < \infty\), and for \(j\) large enough:

\[
0 < \mathcal{F}_{L_{k_j}}(n_{k_j}, p_{k_j}) < \liminf_{j \to \infty} \mathcal{F}_{L_{k_j}}(n_{k_j}, p_{k_j}) + 1 = M,
\]

which implies \((n_{k_j}, p_{k_j}) \in H^1(D; S^2) \times H^1(D; S^2)\).

Proceeding as in the proof of Proposition 3, we can find another subsequence \((n_{k_{j_l}}, p_{k_{j_l}})\) which converges in \(L^1\) to an element \((n_*, p_*)\) in \(Y_2\). By uniqueness of limit, we conclude that \((n, p) = (n_*, p_*) \in Y_2\) and

\[
\lim_{L \to \infty} \mathcal{F}_{L_{k_{j_l}}}(n_{k_{j_l}}, p_{k_{j_l}}) = \liminf_{j \to \infty} \mathcal{F}_{L_{k_j}}(n_{k_j}, p_{k_j}).
\]

Therefore, we have reduced our task to prove that if \((n, p) \in Y_2\) and \(\{n_k, p_k\} \subset (H^1(D; S^2) \times H^1(D; S^2)) \cap X\) is such that \((n_k, p_k) \to (n, p)\) in \(L^1\), and \(0 < \mathcal{F}_{L_k}(n_k, p_k) \leq M < \infty\) then \(\liminf_{L \to \infty} \mathcal{F}_{L_k}(n_k, p_k) \geq \mathcal{F}_\infty(n, p)\).

Given \((n, p) \in Y_2\), we denote by \(N\) the total number of jump discontinuities of \(n_1\) and \(p_2\) counted once. Since \(S(p_2) = 2\) for elements in \(Y_2\), we know that \(N \geq 2\), while from \(n_1 \in BV_r(D; \{-\sin \theta_B, \sin \theta_B\})\) we have \(2 \leq N < \infty\).

Let \(0 = \theta_1 < ... < \theta_j < ... < \theta_{N+1} = 1\) be the points of discontinuity, we observe that if \(1 < j < N\) only \(n_1\) has a jump at \(\theta_j\), and at \(j = 1, N\) \(p_1\) is discontinuous while \(n_1\) might or might not be discontinuous.

By passing to a subsequence if necessary, we can assume pointwise convergence a.e., and for any \(\eta \in (0, \sin \theta_B)\) we can find \(\delta_1^j, \delta_2^j\) such that \(\theta_j - \delta_1^j, \theta_j + \delta_2^j\) are points of convergence for \(n_k\) and \(p_k\), and the intervals \(I_j = (\theta_j - \delta_1^j, \theta_j + \delta_2^j)\) are disjoint. Then, since \(N < \infty\), for \(k\) large enough, say \(k > k_\eta\), we can assume that the following relations hold for the components of \(n_k\) and \(p_k\):

For \(n_k\):

\[
\sin \theta_B - \eta < (n_1)_k (\theta_j - \delta_1^j) \leq \sin \theta_B
\]

\[
- \sin \theta_B \leq (n_1)_k (\theta_j + \delta_2^j) \leq - \sin \theta_B + \eta
\]

(23)
or

\[-\sin \theta_B \leq (n_1)_k (\theta_j - \delta^1_j) \leq -\sin \theta_B + \eta\]
\[\sin \theta_B - \eta \leq (n_1)_k (\theta_j + \delta^2_j) \leq \sin \theta_B,\]  
(24)

if \(1 < j < N\), and

\[(n_1)_k (\theta_1 - \delta^1_1) = \sin \theta_B\]
\[n_1(0^+) \leq (n_1)_k (\theta_1 + \delta^2_1) \leq n_1(0^+) + \eta,\]  
(25)

if \(j = 1\), and

\[(n_1)_k (\theta_N + \delta^2_N) = \sin \theta_B\]
\[n_1(1^-) \leq (n_1)_k (\theta_N - \delta^1_N) \leq n_1(1^-) + \eta.\]  
(26)

for \(j = N\). Which also imply, using the constraints \(|n_k| = 1\), and \((n_3)_k = \cos \theta_B:\)

\[-\eta_0 \leq (n_2)_k (\theta_j - \delta^1_j) \leq \eta_0,\]
\[-\eta_0 \leq (n_2)_k (\theta_j + \delta^2_j) \leq \eta_0,\]  
(27)

with \(\eta_0 \to 0\) as \(\eta \to 0\).

For \(p_k:\)

\[-\eta < (p_1)_k (\theta_j - \delta^1_j) < \eta, \quad -\eta < (p_1)_k (\theta_j + \delta^2_j) < \eta,\]
\[-\eta < (p_3)_k (\theta_j - \delta^1_j) < \eta, \quad -\eta < (p_3)_k (\theta_j + \delta^2_j) < \eta,\]
\[-\eta < (p_2)_k (\theta_j - \delta^1_j) < 1, \quad 1 - \eta < (p_2)_k (\theta_j + \delta^2_j) < 1,\]  
(28)

if \(1 < j < N\), and

\[(p_1)_k (\theta_1 - \delta^1_1) = 0, \quad -\eta < (p_1)_k (\theta_1 + \delta^2_1) < \eta,\]
\[(p_3)_k (\theta_1 - \delta^1_1) = 0, \quad -\eta < (p_3)_k (\theta_1 + \delta^2_1) < \eta,\]
\[(p_2)_k (\theta_1 - \delta^1_1) = -1, \quad 1 - \eta < (p_2)_k (\theta_1 + \delta^2_1) < 1,\]  
(29)

if \(j = 1\), and

\[-\eta < (p_1)_k (\theta_N - \delta^1_N) < \eta, \quad (p_1)_k (\theta_N + \delta^2_N) = 0,\]
\[-\eta < (p_3)_k (\theta_N - \delta^1_N) < \eta, \quad (p_3)_k (\theta_N + \delta^2_N) = 0,\]
\[-\eta < (p_2)_k (\theta_N - \delta^1_N) < 1, \quad (p_2)_k (\theta_N + \delta^2_N) = -1,\]  
(30)

if \(j = N\).

Therefore, up to subsequences, for \(k > k_n\), starting from

\[
\mathcal{F}_{L_k} (n_k, p_k) \geq \sum_{j=2}^{N-1} \frac{1}{L_k} \left[ \frac{1}{2} k_n^* \int_{i_j} |\nabla n_k|^2 dx + \frac{1}{2} k_p^* \int_{i_j} |\nabla p_k|^2 dx \right]
\[+ L_k \int_{i_j} p_1^2 dx + \frac{1}{2} k_{np} \int_{i_j} p_2^2 dx + \frac{1}{2} k_E \int_{i_j} [p_1^2 + (p_2 - 1)^2 + p_3^2] dx \right].
\]
and denoting $T_j = L_k \delta_j$, where $\delta_j = \frac{\delta^2 + \delta^1}{2}$, the change of variable $x = \frac{1}{L_k} s + \theta_j + \frac{\delta^2 - \delta^1}{2}$ gives:

$$F_{L_k}(n_k, p_k) \geq \sum_{j=2}^{N-1} \int_{-T_j}^{T_j} E(w_{j,k}, z_{j,k}) \, dx + \int_{-T_1}^{T_1} E(w_{1,k}, z_{1,k}) \, dx$$

$$+ \int_{-T_N}^{T_N} E(w_{N,k}, z_{N,k}) \, dx,$$

(31)

with $w_{j,k}, z_{j,k} \in H^1((-T_j, T_j); S^2)$, $w_{j,k} \cdot z_{j,k} = 0$, $(w_{j,k})_3 = \cos \theta_B$, and where at $\pm T_j$ the functions $(w_{j,k}, z_{j,k})$ verify conditions (23) or (24), and (27), (28) if $1 < j < N$, while $(w_{1,k}, z_{1,k})$ verify conditions (25), (27), and (29), and $(w_{N,k}, z_{N,k})$ verify conditions (26), (27), and (30).

Taking the infimum over all functions $w_j, z_j, v, u, v_1, u_1$ verifying the assumptions above, for $k > k_\eta$ we derive:

$$F_{L_k}(n_k, p_k) \geq \inf_{w_j, z_j, v, u, v_1, u_1} \left\{ \sum_{j=2}^{N-1} \int_{-T_j}^{T_j} E(w_j, z_j) \, dx + \int_{-T_1}^{T_1} E(v, u) \, dx \right.$$

$$+ \int_{-T_N}^{T_N} E(v_1, u_1) \, dx \right\}.$$

Additionally, since the limit function $p$ is constant in $I_j$ in both (23) and (24), by symmetry we can fix one of the two conditions, say (24), and conclude, for all $k > k_\eta$, that:

$$F_{L_k}(n_k, p_k) \geq \inf \left\{ \sum_{j=2}^{N-1} \int_{-T_j}^{T_j} E(w, z) \, dx + \int_{-T_1}^{T_1} E(v, u) \, dx \right.$$
\[
\begin{align*}
&+ \int_{-T}^{T} E(v_1, u_1) \, dx, \\
&\quad + \inf_{T \geq 0} \left\{ \int_{-T}^{T} E(v, u) \, dx \right\} + \inf_{T \geq 0} \left\{ \int_{-T}^{T} E(v_1, u_1) \, dx \right\},
\end{align*}
\]

(32)

where the first infimum is taken over functions in \(H^1((-T, T); S^2)\), with \(w \cdot z = v \cdot u = v_1 \cdot u_1 = 0\), \((w)_3 = (v)_3 = (v_1)_3 = \cos \theta_B\), and where at \(\pm T\) the functions \((w, z)\) verify condition (24), (27), and (28), while \((v, u)\) verify conditions (25), (27), and (29), and \((v_1, u_1)\) verify conditions (26), (27), and (30), all of which we remind the reader depend on \(\eta\), letting \(\eta \to 0\) we obtain:

\[
\lim_{L_k \to \infty} \inf \mathcal{F}_{L_k}(n_k, p_k) \geq \mathcal{F}_\infty(n, p).
\]

**Limsup Inequality:** We need to show that for every \((n, p) \in X\) there exists \(\{(n_k, p_k)\} \subset X\) such that \((n_k, p_k)\) converges in \(L^1\) and

\[
\lim_{L_k \to \infty} \sup \mathcal{F}_{L_k}(n_k, p_k) \leq \mathcal{F}_\infty(n, p).
\]

Let \((n, p) \in X\), if \((n, p) \in X \backslash Y_2\) then \(\mathcal{F}_\infty(n, p) = \infty\), and we set \((n_k, p_k) = (n, p)\) for all \(k\).

If \((n, p) \in Y_2\) instead, then \(\mathcal{F}_\infty(n, p) < \infty\), that is \(\mathcal{F}(n, p) < \infty\). Let \(N\) be the total number of points of discontinuity of \(n_1\) and \(p_2\) counted once.

By the definition of \(\mathcal{F}(n, p)\), for any \(k > 0\), there exists \(T_1, T_2, T_3\) and \(w, z \in H^1((-T_1, T_1); S^2)\), \(v, u \in H^1((-T_2, T_2); S^2)\) and \(v_1, u_1 \in H^1((-T_3, T_3); S^2)\), with suitable boundary conditions, such that

\[
(N - 2) \int_{-T_1}^{T_1} E(w, z) \, dx + \int_{-T_2}^{T_2} E(v, u) \, dx + \int_{-T_3}^{T_3} E(v_1, u_1) \, dx \leq \mathcal{F}(n, p) + \frac{1}{k}.
\]

We let \(0 = \theta_1 < \theta_2 < \ldots < \theta_N = 1\) denote the points of discontinuity. Note that \(T_1, T_2, T_3\) and all the functions above depend on the choice of \(k\).

We next pick \(L_k > k\) large enough so to have:

\[
0 < \frac{2T_3}{L_k} < \theta_2 - \frac{T_2}{L_k} < \theta_2 + \frac{T_2}{L_k} < \theta_3 - \frac{T_3}{L_k} < \ldots < \theta_{N-1} + \frac{T_3}{L_k} < 1 - \frac{2T_3}{L_k} < 1,
\]

and define:

\[
n_k(x) = \begin{cases} 
    v(L_k(x - \frac{T_2}{L_k})) & \text{if } 0 \leq x \leq \frac{2T_2}{L_k}, \\
    w(\pm L_k(x - \theta_j)) & \text{if } \theta_j - \frac{T_j}{L_k} \leq x \leq \theta_j + \frac{T_j}{L_k}, \quad j = 2, \ldots, N - 1, \\
    v_1(L_k(x + \frac{T_3}{L_k} - 1)) & \text{if } 1 - \frac{2T_3}{L_k} \leq x \leq 1, \\
    n(x) & \text{otherwise}.
\end{cases}
\]

(33)

We also consider an analogous definition for \(p_k(x)\).

As in [2], we remark that the choice between the plus and minus sign in (33) can be made in such a way that the resulting function is continuous, and the sequence \((n_k, p_k)\) is an element of \(X\). It is also a consequence of its definition that the sequence converges in \(L^1\) to \((n, p)\).
The energy of an element \((n_k, p_k)\) of the sequence is

\[
\mathcal{F}_{L_k} (n_k, p_k) = \frac{2\pi^2}{L_k} \int_0^{\frac{2\pi}{L_k}} \left( \frac{k_n^*}{2L_k} |\nabla n_k|^2 + \frac{1}{2} \frac{k_p^*}{L_k} |\nabla p_k|^2 + L_k(p_k)^2 \right) + \frac{1}{2} L_k k_n p_n (p_k)_2^2
\]

\[
+ \frac{1}{2} L_k |k_E| \left[ ((p_k)_1^2 + ((p_k)_2 - 1)^2 + (p_k)_3^2) \right) dx
\]

\[
+ \sum_{j=2}^{N-2} \int_{\theta_j - \frac{T_1}{L_k}}^{\theta_j + \frac{T_1}{L_k}} \left( \frac{k_n^*}{2L_k} |\nabla n_k|^2 + \frac{1}{2} \frac{k_p^*}{L_k} |\nabla p_k|^2 + L_k(p_k)^2 \right) + \frac{1}{2} L_k k_n p_n (p_k)_3^2
\]

\[
+ \frac{1}{2} L_k |k_E| \left[ ((p_k)_1^2 + ((p_k)_2 - 1)^2 + (p_k)_3^2) \right) dx
\]

\[
+ \int_{1 - \frac{2\pi}{L_k}}^{\frac{2\pi}{L_k}} \left( \frac{k_n^*}{2L_k} |\nabla n_k|^2 + \frac{1}{2} \frac{k_p^*}{L_k} |\nabla p_k|^2 + L_k(p_k)^2 \right) + \frac{1}{2} L_k k_n p_n (p_k)_3^2
\]

where the other parts of the integral are zero since \(n_k = n\) constant, \(p_k = p\) constant, and \(p_1 = p_3 = 0, p_2 = 1\) between singularities.

If we now make the changes of variables:

\[
s = L_k \left( x - \frac{T_1}{L_k} \right) \quad \text{on} \quad \left[ 0, \frac{2\pi}{L_k} \right],
\]

\[
s = \pm L_k \left( x - \frac{T_1}{L_k} \right) \quad \text{on} \quad \left[ \theta_j - \frac{T_1}{L_k}, \theta_j + \frac{T_1}{L_k} \right],
\]

\[
s = L_k \left( x + \frac{T_1}{L_k} - 1 \right) \quad \text{on} \quad \left[ 1 - \frac{2\pi}{L_k}, 1 \right],
\]

we obtain:

\[
\mathcal{F}_{L_k} (n_k, p_k) = (N - 2) \int_{-T_1}^{T_1} E(w, z) ds + \int_{-T_2}^{T_2} E(v, u) ds + \int_{-T_3}^{T_3} E(v_1, u_1) ds
\]

\[
\leq \mathcal{F}(n, p) + \frac{1}{k},
\]

and by taking the lim sup for \(k \to \infty\), recalling that we picked \(L_k > k\), we gather

\[
\limsup_{L_k \to \infty} \mathcal{F}_{L_k} (n_k, p_k) \leq \mathcal{F}(n, p).
\]

5. Minimizers of \(\Gamma\)-limit. In this section, we study the minimizers of the limiting functional \(\mathcal{F}_\infty\) in (18), here we are interested in their behavior as functions of the physical parameters.

We remark that existence of minimizers for this functional is a consequence of the \(\Gamma\)-limit procedure, since the \(\Gamma\)-limit as defined in the previous section is always lower semicontinuous in \(X\).

The energy \(\mathcal{F}_\infty\) of an element \((n, p)\) in \(X\) is unbounded unless \((n, p) \in Y_2\), therefore we can restrict our attention to elements in \(Y_2\). If, as mentioned in the previous section, we think of \(BV_{\text{loc}}(D; (-\sin \theta_B, \sin \theta_B))\) as the space of functions \(v\) in \(BV_{\text{loc}}(\mathbb{R})\) such that \(v \equiv \sin \theta_B\) on \((-\infty, 0) \cup (1, \infty)\), for \((n, p) \in Y_2\) we have that
$n_1$ has one of four fundamental behaviors described for simplicity via the graphs presented in Figure 5.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{Possible behaviors near the boundary of the component $n_1$ of $(n, p) \in Y_2$.}
\end{figure}

As a consequence, we claim that there are only two candidates for minimizers of $F_\infty$, namely, $(n_c, p_d)$ and $(n_d, p_d)$, where

\begin{align*}
  n_c(x) &= (\sin \theta_B, 0, \cos \theta_B) & \text{if } x \in (0, 1), \\
  n_d(x) &= (-\sin \theta_B, 0, \cos \theta_B) & \text{if } x \in (0, 1), \\
  p_d(x) &= (0, 1, 0) & \text{if } x \in (0, 1),
\end{align*}

and

\begin{align*}
  n_c(0) &= n_c(1) = n_d(0) = n_d(1) = (\sin \theta_B, 0, \cos \theta_B), \\
  p_d(0) &= p_d(1) = (0, -1, 0).
\end{align*}

This can be justified, by noticing that if $(n, p) \neq (n_d, p_d)$ is of Type I then $F_\infty(n_d, p_d) < F_\infty(n, p)$, while if $(n, p) \neq (n_c, p_d)$ is of Type II then $F_\infty(n_c, p_d) < F_\infty(n, p)$, and, finally, that if $(n, p)$ is of Type III and $(\tilde{n}, \tilde{p})$ is of Type IV, then $\min \{F_\infty(n_c, p_d), F_\infty(n_d, p_d)\} < \min \{F_\infty(n, p), F_\infty(\tilde{n}, \tilde{p})\}$. These inequalities are all true since for $(n_c, p_d)$ and $(n_d, p_d)$ one has $N = 2$, and the last two infima in the definition of $F$ depend only on the behavior of the functions near the boundary.

To determine the minimizers of $F_\infty$, we then need to compare the energies of $(n_c, p_d)$ and $(n_d, p_d)$, which for these states simplify to:

\begin{equation}
  \inf_{T \geq 0} \left\{ \int_{-T}^{T} E(v, u) \, dx \right\} + \inf_{T \geq 0} \left\{ \int_{-T}^{T} E(v_1, u_1) \, dx \right\},
\end{equation}

(36)
for \(v, u, v_1, u_1 \in H^1((-T, T); S^2)\) such that
\[
  v(\pm T) = (n_1(0^\pm), 0, \cos \theta_B), \quad v_1(\pm T) = (n_1(1^\pm), 0, \cos \theta_B),
\]
\[
  u(\pm T) = (0, \pm 1, 0), \quad u_1(\pm T) = (0, \mp 1, 0),
\]
\[
  v \cdot u = 0 = v_1 \cdot u_1, \quad v_3 = (v_1)_3 = \cos \theta_B.
\]  
(37)

Furthermore, if we fix either \((n_c, p_d)\) or \((n_d, p_d)\), it’s straightforward to see that given \((v, u)\) verifying the relevant conditions in (37), if we consider \(v_1(s) := v(-s)\)
and \(u_1(s) := u(-s)\), then \(v_1, u_1\) will verify the analogous conditions in (37), and
\[
  E(v, u) = E(v_1, u_1).
\]  
In a similar way, given a \((v_1, u_1)\) we can build an admissible \((v, u)\) with same energy \(E\), and we can conclude that the two infima in equation (36) are equal.

A summary of our discussion can be express in the form of the energies for our
two candidates minimizers: \(F_\infty(n_c, p_d) = 2\inf_{T \geq 0} \left\{ \int_{-T}^{T} E(v, u) \, dx \right\}\), for \(v, u \in H^1((-T, T); S^2)\) with
\[
  v(\pm T) = (\sin \theta_B, 0, \cos \theta_B),
\]
\[
  u(\pm T) = (0, \pm 1, 0),
\]
\[
  v \cdot u = 0, \quad v_3 = \cos \theta_B,
\]  
(38)
and, \(F_\infty(n_d, p_d) = 2\inf_{T \geq 0} \left\{ \int_{-T}^{T} E(v, u) \, dx \right\}\), for \(v, u \in H^1((-T, T); S^2)\) with
\[
  v(\pm T) = (\pm \sin \theta_B, 0, \cos \theta_B),
\]
\[
  u(\pm T) = (0, \pm 1, 0),
\]
\[
  v \cdot u = 0, \quad v_3 = \cos \theta_B.
\]  
(39)

At first sight one might think that the state with continuous \(n_1\) component, that
is \((n_c, p_d)\), might provide the least energy, but a careful examination of the terms
involved shows that the relative size of the physical parameters will play a role, as
displayed in the following result.

Proposition 4. For fixed \(k_E, k_n^*,\) and \(k_p^*\), if \(k_n^* \geq k_p^*\) there exists \(c_0 > 0\) such that
for any \(k_{np} > c_0\) the global minimizer of \(F_\infty\) is \((n_d, p_d)\).

Proof. We rewrite the energy in terms of the angles introduced in equation (1),
where we notice that in here we are considering \(\Delta = 0\) and \(\theta = \theta_B\), so that if
\(|v| = |u| = 1, v \cdot u = 0, \) and \(v_3 = \cos \theta_B\), we have:
\[
  v = \langle \sin \theta_B \cos \phi, \sin \theta_B \sin \phi, \cos \theta_B \rangle;
\]
\[
  u = \langle \sin \alpha \cos \theta_B \cos \phi + \sin \phi \cos \alpha, \sin \alpha \cos \theta_B \sin \phi - \cos \phi \cos \alpha,\n\]
\[\quad - \sin \alpha \sin \theta_B \rangle,
\]
and, we can rewrite
\[
  \int_{-T}^{T} E(v, u) \, dx = \int_{-T}^{T} \left[ \frac{1}{2} (k_n^* \sin^2 \theta_B + k_p^* \cos^2 \theta_B + k_n^* \sin^2 \theta_B \cos^2 \alpha) (\phi')^2 \right.
\]
\[ + \frac{1}{2} k_p^* (\alpha')^2 + k^*_p \cos \theta_B (\alpha' \phi') \]
\[ + \left( 1 + \frac{|k_E|}{2} \right) (\sin \alpha \cos \theta_B \cos \phi + \sin \phi \cos \alpha)^2 \]
\[ + \left( \frac{1}{2} k_{np} + \frac{|k_E|}{2} \right) \sin^2 \alpha \sin^2 \theta_B \]
\[ + \frac{|k_E|}{2} (\sin \alpha \cos \theta_B \sin \phi - \cos \phi \cos \alpha - 1)^2 \right) \] dx. \quad (40)

The boundary conditions in (38) and (39) translate to
\[ \alpha(-T) = 0, \quad \alpha(T) = \pi, \]
\[ \phi(-T) = 0 = \phi(T), \quad (41) \]
and
\[ \alpha(-T) = 0 = \alpha(T), \]
\[ \phi(-T) = 0, \quad \phi(T) = \pi, \quad (42) \]
respectively.

We use the assumption \( k_{n}^* \geq k_{p}^* \) to rewrite (40):
\[
\int_{-T}^{T} \left[ \frac{1}{2} k_{p}^* \sin^2 \theta_B (\alpha')^2 + \left( \frac{1}{2} k_{np} + \frac{|k_E|}{2} \right) \sin^2 \alpha \sin^2 \theta_B \right. \\
\left. + \frac{k_{p}^*}{2} (\cos \theta_B \alpha' + \phi')^2 + \frac{1}{2} \left( k_{n}^* - k_{p}^* \right) \sin^2 \theta_B + \frac{1}{2} k_{p}^* \sin^2 \theta_B \cos^2 \alpha \right] (\phi')^2 \\
\left. + \left( 1 + \frac{|k_E|}{2} \right) (\sin \alpha \cos \theta_B \cos \phi + \sin \phi \cos \alpha)^2 \\
\right. \\
\left. + \frac{|k_E|}{2} (\sin \alpha \cos \theta_B \sin \phi - \cos \phi \cos \alpha - 1)^2 \right) \] dx. \quad (43)

and by a standard procedure, we find a lower bound for the energy of \((n_c, p_d)\):
\[
\mathcal{F}_\infty (n_c, p_d) \geq 2 \int_{-T}^{T} \left[ \frac{1}{2} k_{p}^* \sin^2 \theta_B (\alpha')^2 + \left( \frac{1}{2} k_{np} + \frac{|k_E|}{2} \right) \sin^2 \alpha \sin^2 \theta_B \right] dx \\
\geq 2 \sin^2 \theta_B \sqrt{k_{p}^* (k_{np} + |k_E|)} \int_{-T}^{T} \sin \alpha \alpha' dx \\
= 4 \sin^2 \theta_B \sqrt{k_{p}^* (k_{np} + |k_E|)}, \quad (44)
\]
where we used in an essential way the boundary condition (41).

To find an upper bound for \(\mathcal{F}_\infty (n_d, p_d)\), we just consider the linear interpolation between the boundary values, and pick \( \alpha(x) \equiv 0, \phi(x) = \frac{\pi}{T} x + \frac{\pi}{2} \).
This choice yields:

\[
F_\infty(n_d, p_d) \leq 2 \inf_{T > 0} \int_{-T}^{T} \left[ \frac{1}{2} \left( k_n^* \sin^2 \theta_B + k_p^* \right) \left( \frac{\pi}{2T} \right)^2 + \left( 1 + \frac{|k_E|}{2} \right) \sin^2 \left( \frac{\pi}{2T} x + \frac{\pi}{2} \right) + \left( \cos \left( \frac{\pi}{2T} x + \frac{\pi}{2} \right) + 1 \right)^2 \right] dx
\]

\[
= 2 \inf_{T > 0} \left\{ \frac{\pi^2}{2T} \left[ \frac{1}{2} \left( k_n^* \sin^2 \theta_B + k_p^* \right) \right] + \left( 1 + \frac{|k_E|}{2} \right) T + \frac{|k_E|}{2} \right\}
\]

\[
= 2 \inf_{T > 0} \left\{ \frac{\pi^2}{4} \left( k_n^* \sin^2 \theta_B + k_p^* \right) \frac{1}{T} + (1 + 2|k_E|) T \right\},
\]

which, taking the infimum over \( T > 0 \), results in to the bound:

\[
F_\infty(n_d, p_d) \leq 4 \sqrt{\frac{\pi^2}{4} \left( k_n^* \sin^2 \theta_B + k_p^* \right) (1 + 2|k_E|)}. \quad (45)
\]

Comparing (44) and (45), we have that \( F_\infty(n_d, p_d) < F_\infty(n_c, p_d) \), for \( k_{np} \) large enough. The discussion proceeding the statement of this proposition implies that \( (n_d, p_d) \) is the global minimizer for such \( k_{np} \) values.

**Remark 2.** As a final remark, we should explain why we claim that the state \( (n_c, p_d) \) represents rotation around the molecular axis, while \( (n_d, p_d) \) suggests rotation around the tilt cone. Looking at the boundary conditions (38), expressed as (41) via the polar angle \( \alpha \) and the azimuthal angle \( \phi \), we see that \( \alpha \) is changing from 0 to \( \pi \), while \( \phi \) is fixed at 0, that is the molecule is rotating around its axis while preserving its position on the tilt cone. Similarly, looking at the boundary conditions (39) in the energy of \( (n_d, p_d) \) as given in (42), we see that now is the azimuthal angle which is changing from 0 to \( \pi \), while the polar angle is fixed at 0, suggesting that the molecule is rotating around the tilt cone, while the relative position of \( n \) and \( p \) remains unchanged.

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