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Dimensional Reduction for the Ferroelectric Smectic A-Type Phase of Bent-Core Liquid Crystals

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Abstract
We analytically derive and numerically simulate a two-dimensional energy functional modelling the effects of a constant electric field on a thin sample of a bent-core liquid crystal in the ferromagnetic SmA-like phase. We start from a three-dimensional domain and show that under proper rescaling and in the limit of small thickness the electric self-interactions term gives rise to boundary terms. We compare our results to previously proposed models.

Keywords Dimensional reduction · Γ-convergence · Bent-core liquid crystals

Mathematics Subject Classification 35J08 · 76A15

1 Introduction

Ferroelectric liquid crystals made of achiral molecules have been extensively studied (Niori et al. 1996; Eremin and Jákli 2013; Jakli et al. 2018), due to their properties of technological interest and their lower production costs. In materials with rod-like molecules, ferroelectricity generally requires molecular chirality coupled with director

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tilt with respect to the smectic layer. Instead, achiral materials composed of bow-like shaped molecules, so-called bent-core liquid crystals (BLCs), might exhibit spontaneous polarization in the non-tilted Smectic A phase (SmA) Niori et al. (1996), resulting from the efficient packing of their bow-shaped molecules, which gives rise to a polar order along the kink direction of the molecules.

While different types of tilted bent-core smectic phases have been known and investigated for the past several decades, orthogonal bent-core smectic phases with ferroelectric properties have been reported only since around 2010. Experimental evidence of such a phase, here denoted by SmAP_{F}, is presented in Reddy et al. (2011), Guo et al. (2011). In Zhu et al. (2012), the authors report a BLC compound exhibiting a SmAP_{F} phase at a lower temperature and a polarization splay-modulated orthogonal phase ($\text{SmAP}_{\text{Fmod}}$) at a higher temperature. The relatively high dielectric constant shown in the SmAP_{F} phase Guo et al. (2011) and the bistable response observed in the $\text{SmAP}_{\text{Fmod}}$ phase Zhu et al. (2012) suggest that orthogonal smectic phase of BLCs may be a good candidate for future competitive optical devices Korblova et al. (2017).

A mathematical challenge faced when modeling and analyzing ferroelectric materials comes from the nonlocal nature of the electric self-interactions. In Bailey et al. (2007), Bailey et al. study the stability of B7 fibers by showing that the concentric cylindrical smectic layers form freestanding fibers with a tilted smectic phase of BLCs. In their work, an expression for the electric self-interactions energy density is provided and used in a one-dimensional radial setting. This energy density consists of three terms: the dielectric interaction with the electric field created by the diverging spontaneous polarization, the dielectric interaction with the external electric field, and their interaction with the spontaneous polarization, see (8). Under some assumptions, such as constant nematic director and fixed smectic layers, and with $\mathbf{p}_h : \Omega_h \to \mathbb{S}^2$ denoting the polarization director, $\Omega_h = (0,1)^2 \times (0,h)$ the material sample, and h the ratio of the film thickness to the film's in-plane length, we arrive at the following dimensionless equation for the electric potential:

$$\nabla \cdot \left(\varepsilon_h^*(\mathbf{p}_h)\, \nabla \Phi_h\right) = \nabla \cdot (\mathbf{p}_h \chi_{\Omega_h}) \quad \text{in } \mathbb{R}^3,$$

where the dielectric tensor $\varepsilon_h^*(\mathbf{p}_h)$ takes possibly different values inside and outside of the domain:

$$\varepsilon_h^*(\mathbf{p}) = \begin{cases} \hat{\varepsilon}(\mathbf{p}) & \text{in } \Omega_h \\ I & \text{outside } \Omega_h, \end{cases}$$

see (3). To model the elastic effects, we start from the elastic free energy proposed in Stallinga and Vertogen (1994), see also Vaupotič et al. (2014). In the end, we arrive to the total free energy for the SmAP_{F} given in non-dimensional form by (17) augmented by (18).

We are interested in deriving a reduced two-dimensional model to study thin samples. In particular, we show that in the thin-film limit setting an appropriately rescaled version of the three-dimensional ferroelectric orthogonal BLCs model described by (17)–(18) leads to a two-dimensional local free energy of the form given in (45). A similar nonlocal energy has been obtained and extensively investigated in the field of micromagnetics. In particular, Kohn and Slastikov in Kohn and Slastikov (2005) characterize the magnetostatic energy for micromagnetics in a thin film with a smooth cross section as a two-dimensional, local limiting variational problem. Our approach is inspired by their work, which we extend fully to the case of a constant coefficient dielectric tensor and a rectangular cross section, and partially to the case of a bounded and measurable coefficient dielectric tensor, which does not dependent on the polarization vector. In Sect. 2, we derive the three-dimensional free energy model, and in Sect. 3 we obtain bounds for its various terms, under some assumptions on the form of the dielectric tensor. We then present a reduced local two-dimensional energy, see (45), motivated by the Γ-convergence results obtained in Theorem 4.1 of Sect. 4.

A two-dimensional energy of the form (45) was recently used in the one-constant approximation setting, that is when the elastic constants are assumed to be all equal, to study electric field effects on a BLC thin sample in the SmAP$_{\text{Fmod}}$ phase García-Cervera et al. (2020). When a term is introduced to relax the unit length constraint of the polarization director, this energy resembles the Ginzburg–Landau functional of superconductivity, with surface energy density given by $(\mathbf{p} \cdot \nu)^2$, on the top and bottom parts of a rectangular domain. In here, we show that in fact this surface energy models the contribution of the nonlocal electric self-interactions. According to the analytical results obtained in García-Cervera et al. (2020), energy minimizing configurations develop a pair of boundary defects, on the top and bottom parts of the boundary, each with $\pm 1/2$ degree. Furthermore, numerical simulations exploring the switching mechanism obtained by reversing the direction of an applied electric field indicate the strong bistability of the SmAP$_{\text{Fmod}}$ bent-core liquid crystals and show that a pair of interior vortices nucleate from the boundary vortex pair, move to the center of the domain, and then annihilate each other.

In Sect. 5, we numerically compare the SmAP$_{\text{Fmod}}$ phase studied in García-Cervera et al. (2020) with the SmAP$_{\text{F}}$ one, by considering gradient flow numerical simulations of a relaxation of the polarization director unit length constraint of the two-dimensional energy (45) applied to model the SmAP$_{\text{F}}$ phase. Our study is consistent with the one-dimensional results for SmAP$_{\text{F}}$ presented in Gornik et al. (2014), Gornik and Vaupotič (2014), Guo et al. (2011). In our two-dimensional confined geometry, when an electric field is applied in the upward direction, a pair of boundary vortices appears on the vertical sides of the domain and move with the electric field, resulting in an upward polarization in most of the domain, see Fig. 1.

To gain a complete picture of the switching mechanism, we also numerically study the non-equal elastic constant model for the SmAP$_{\text{Fmod}}$ phase. In contrast with the results for the one-constant approximation obtained in García-Cervera et al. (2020), only one interior vortex appears near one of the boundary vortices, the interior vortex then moves toward the opposite boundary vortex to complete the switching, see Fig. 2, this picture is consistent with the scenario proposed in Zhu et al. (2012).

Notations:

(i) For $a > 0, b > 0$, we denote $\Omega_b^a = (0, a)^2 \times (0, b)$;
(ii) For $b > 0$, we let $\Omega_b \equiv \Omega_b^1 = (0, 1)^2 \times (0, b)$;
(iii) If $\mathbf{p} = (p_1, p_2, 0)$, we denote $\mathbf{p}^\perp = (-p_2, p_1, 0)$;

(iv) Given $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ and $\mathbf{p}(\mathbf{x}) = (p_1(\mathbf{x}), p_2(\mathbf{x}), p_3(\mathbf{x}))$, we define $\mathrm{div}'\mathbf{p} = \partial_1 p_1 + \partial_2 p_2$, $\mathrm{curl}'\mathbf{p} = \partial_1 p_2 - \partial_2 p_1$, and $|\nabla'\mathbf{p}|^2 = \sum_{i=1}^2 \sum_{j=1}^3 (\partial_i p_j)^2$;

(v) For $\mathbf{p}_b : \Omega_b \to \mathbb{R}$, we let $\widetilde{\mathbf{p}}_b : \Omega_1 \to \mathbb{R}$ be the rescaling of $\mathbf{p}_b$ in the x_3 variable, that is $\widetilde{\mathbf{p}}_b(x_1, x_2, x_3) = \mathbf{p}_b(x_1, x_2, b\,x_3)$, and $\overline{\mathbf{p}}_b : (0,1)^2 \to \mathbb{R}$ the average of $\mathbf{p}_b$ over $(0, b)$, that is $\overline{\mathbf{p}}_b(x_1, x_2) = \frac{1}{b}\int_0^b \mathbf{p}_b(x_1, x_2, x_3)\, dx_3$, whenever the integral exists. A change of variables shows that

$$\overline{\mathbf{p}}_b(x_1, x_2) = \int_0^1 \widetilde{\mathbf{p}}_b(x_1, x_2, x_3)\, dx_3. \tag{1}$$

(vi) By L_c^∞ we denote the set of L^∞ functions with compact support.

2 Three-Dimensional Model

Bent-core liquid crystal molecules can be described using two orthogonal unit vectors: $\mathbf{n}$ and $\mathbf{p}$, with $|\mathbf{n}| = |\mathbf{p}| = 1$ and $\mathbf{n} \cdot \mathbf{p} = 0$. The so-called nematic director $\mathbf{n}$ is parallel to the axis of the molecule, while $\mathbf{p}$, known as polarization director, points in the direction of the bow of the molecule. Since the polarization director $\mathbf{p}$ follows the bent of the molecule, its direction is physically relevant, unlikely for the nematic director $\mathbf{n}$ where in fact the unit vectors $\pm\mathbf{n}$ are physically equivalent. According to the physics literature, $\mathbf{p}$ is also in the same direction as the spontaneous polarization $\mathbf{P}$, which can then be written as $\mathbf{P} = P_0\,\mathbf{p}$ with $P_0 > 0$. In the SmA phase a material forms layers, which are locally perpendicular to the nematic director $\mathbf{n}$. The layer structure can be described by a complex order parameter ψ. We consider a sample in the shape of a parallelepiped with a square base of length side L and height t: $\Omega_t^L = (0, L)^2 \times (0, t)$. Since we are interested in the regime where the smectic layers are well-defined, we assume the smectic order parameter ψ, the intensity of the spontaneous polarization P_0, and the nematic director $\mathbf{n}$ to be constants. We take $\mathbf{n}$ oriented in the z-direction, $\mathbf{n} = \mathbf{e}_3$, namely we assume fixed smectic layers parallel to the xy-plane. By the orthogonality constraint this last assumption implies that $\mathbf{p}$ has only two nonzero components:

$$\mathbf{p} = (p_1, p_2, 0). \tag{2}$$

Because all the terms in the energy density involving the smectic order parameter ψ are constant, we will neglect them. Both polarization and nematic directors are defined only in the liquid crystal sample. However, in the following, when needed, we will implicitly consider the directors as defined in the whole space by extending them to zero outside the sample.

We refer to the *cell thickness* as to the dimension of the sample in the z direction (t in our notation above, and in reference Kohn and Slastikov (2005)), and to the *cell size* as to the dimension of the sample in the x and y directions (L in our notation above, and in reference Gornik et al. (2014)).

We include electric self-interactions terms as modeled by Bailey et al. (2007), see also Bauman and Phillips (2012), and elastic contributions as described in the work of Stallinga and Vertogen (1994), see also Longa et al. (1998) and Vaupotič et al.

(2014). The electric self-interactions energy density can be expressed in terms of the electric field induced by the diverging spontaneous polarization E_i, the externally applied electric field E_{ex}, and their interaction with the spontaneous polarization $\mathbf{P}$. If we denote by $\chi_{\Omega_t^L}$, the characteristic function of Ω_t^L, following Bailey et al. (2007), we have:

$$\left(\frac{1}{2}\varepsilon_0 \hat{\varepsilon} E_i \cdot E_i - \mathbf{P} \cdot E_i - \frac{1}{2}\varepsilon_0 \hat{\varepsilon} E_{ex} \cdot E_{ex} - \mathbf{P} \cdot E_{ex}\right) \chi_{\Omega_t^L} \\ + \frac{1}{2}\varepsilon_0 \left(E_i \cdot E_i - E_{ex} \cdot E_{ex}\right) \left(1 - \chi_{\Omega_t^L}\right),$$

where ε_0 is the dielectric permittivity of free space and $\hat{\varepsilon}$ is the relative dielectric tensor of the material. E_i and E_{ex} are defined in the whole space.

In principle, one has $\hat{\varepsilon}(\mathbf{p}) = \varepsilon_p\, \mathbf{p} \otimes \mathbf{p} + \varepsilon_m\, \mathbf{m} \otimes \mathbf{m} + \varepsilon_n\, \mathbf{n} \otimes \mathbf{n}$, where $\mathbf{p}$, $\mathbf{n}$, $\mathbf{m}$ form an orthonormal basis, and ε_p, ε_m and ε_n are positive dimensionless material constants. If $\mathbf{n} = \mathbf{e}_3$, for $\mathbf{m} = (-p_2, p_1, 0)$ this gives

$$\hat{\varepsilon}(\mathbf{p}) = \begin{bmatrix} (\varepsilon_p - \varepsilon_m)\, p_1^2 + \varepsilon_m & (\varepsilon_p - \varepsilon_m)\, p_1\, p_2 & 0 \\ (\varepsilon_p - \varepsilon_m)\, p_2\, p_1 & (\varepsilon_p - \varepsilon_m)\, p_2^2 + \varepsilon_m & 0 \\ 0 & 0 & \varepsilon_n \end{bmatrix}, \tag{3}$$

and, for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$, it holds

$$\begin{aligned} \mathbf{x}^T \hat{\varepsilon}(\mathbf{p})\, \mathbf{y} &= (\varepsilon_p - \varepsilon_m)\, p_1^2\, x_1\, y_1 + \varepsilon_m x_1 y_1 + (\varepsilon_p - \varepsilon_m)\, p_2\, p_1\, x_2\, y_1 \\ &\quad + (\varepsilon_p - \varepsilon_m)\, p_1\, p_2\, x_1\, y_2 + (\varepsilon_p - \varepsilon_m)\, p_2^2\, x_2\, y_2 + \varepsilon_m x_2\, y_2 + \varepsilon_n x_3 y_3 \\ &= \varepsilon_p \left(p_1^2\, x_1\, y_1 + p_2\, p_1 (x_2\, y_1 + x_1\, y_2) + p_2^2\, x_2\, y_2\right) \\ &\quad + \varepsilon_m \left((1 - p_1^2)\, x_1\, y_1 - p_2\, p_1 (x_2\, y_1 + x_1\, y_2) + (1 - p_2^2)\, x_2\, y_2\right) \\ &\quad + \varepsilon_n x_3 y_3 \\ &= \varepsilon_p \left(p_1^2\, x_1\, y_1 + p_2\, p_1 (x_2\, y_1 + x_1\, y_2) + p_2^2\, x_2\, y_2\right) \\ &\quad + \varepsilon_m \left(p_2^2\, x_1\, y_1 - p_2\, p_1 (x_2\, y_1 + x_1\, y_2) + p_1^2\, x_2\, y_2\right) + \varepsilon_n x_3 y_3. \end{aligned}$$

From this, we see that

$$\begin{aligned} \mathbf{x}^T \hat{\varepsilon}(\mathbf{p})\, \mathbf{x} &= \varepsilon_p\, (p_1\, x_1 + p_2\, x_2)^2 + \varepsilon_m\, (p_2\, x_1 - p_1\, x_2\,)^2 + \varepsilon_n x_3^2 \\ &\geq \varepsilon_- \left[(p_1\, x_1 + p_2\, x_2)^2 + (p_2\, x_1 - p_1\, x_2\,)^2 + x_3^2\right], \end{aligned}$$

and

$$\begin{aligned} \mathbf{x}^T \hat{\varepsilon}(\mathbf{p})\, \mathbf{y} &\leq \varepsilon_+ \left(|x_1|\,|y_1| + |x_2|\,|y_2| + |x_3||y_3|\right) + (\varepsilon_p - \varepsilon_m) p_2\, p_1 (x_2\, y_1 + x_1\, y_2) \\ &\leq \varepsilon_+ |\mathbf{x}|\,|\mathbf{y}| + |\varepsilon_p - \varepsilon_m|\,|x_2\, y_1 + x_1\, y_2| \leq \varepsilon_+ \left(|\mathbf{x}|\,|\mathbf{y}| + |x_2\, y_1 + x_1\, y_2|\right) \end{aligned}$$

where $\varepsilon_- = \min\{\varepsilon_p, \varepsilon_m, \varepsilon_n\}$, and $\varepsilon_+ = \max\{\varepsilon_p, \varepsilon_m, \varepsilon_n\}$.

Therefore, we conclude that

$$\mathbf{x}^T \hat{\varepsilon}(\mathbf{p})\, \mathbf{x} \geq \varepsilon_- \, |\mathbf{x}|^2 \quad \text{and} \quad \mathbf{x}^T \hat{\varepsilon}(\mathbf{p})\, \mathbf{y} \leq 2\, \varepsilon_+ \, |\mathbf{x}|\, |\mathbf{y}|. \tag{4}$$

Introducing the electric potential $\nabla \Phi_t^L$, defined as $E_i = -\nabla \Phi_t^L$, Gauss's law yields

$$\varepsilon_0 \, \nabla \cdot \left(\varepsilon^*_{\Omega_t^L}(\mathbf{p}) \, \nabla \Phi_t^L \right) = \nabla \cdot (\mathbf{P} \chi_{\Omega_t^L}) \quad \text{in } \mathbb{R}^3, \tag{5}$$

where

$$\varepsilon^*_{\Omega_t^L}(\mathbf{p}) = \begin{cases} \hat{\varepsilon}(\mathbf{p}) & \text{in } \Omega_t^L, \\ I & \text{outside } \Omega_t^L, \end{cases} \tag{6}$$

with I being the identity tensor. Under our assumptions, if we let $\underline{\epsilon} = \min\{\varepsilon_-, 1\}$, and $\overline{\epsilon} = \max\{2\, \varepsilon_+, 1\}$, given any $\mathbf{p}$ and $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$, regardless of the values of L and t, we have

$$\mathbf{x}^T \varepsilon^*_{\Omega_t^L}(\mathbf{p})\, \mathbf{x} \geq \underline{\epsilon}\, |\mathbf{x}|^2; \qquad \mathbf{x}^T \varepsilon^*_{\Omega_t^L}(\mathbf{p})\, \mathbf{y} \leq \overline{\epsilon}\, |\mathbf{x}|\, |\mathbf{y}|. \tag{7}$$

For a constant applied electric field, the terms that contain just E_{ex} are constants, and we are led to consider the following electric self-interactions energy density f_{el}:

$$f_{el} = (-\mathbf{P} \cdot E_i - \mathbf{P} \cdot E_{ex})\, \chi_{\Omega_t^L} + \frac{1}{2} \varepsilon_0 \varepsilon^*_{\Omega_t^L}(\mathbf{p})\, E_i \cdot E_i, \tag{8}$$

together with (5).

Our convergence results apply generally to the case of a relative dielectric tensor $\hat{\varepsilon}(\mathbf{x})$ that is independent of $\mathbf{p}$. In particular, we obtain a general Γ-convergence result along subsequences (see Theorem 4.1, Case I below). For the simplified case, when the dielectric tensor is a constant diagonal matrix we obtain a stronger, more explicit, Γ-convergence result (see Theorem 4.1, Case II below). Note that in Bauman et al. Bauman and Phillips (2012) the relative dielectric tensor $\hat{\varepsilon}(\mathbf{x})$ is taken to be a constant diagonal matrix.

$$\hat{\varepsilon}(\mathbf{p}) \equiv \hat{\varepsilon}_c = \begin{bmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_3 \end{bmatrix}, \tag{9}$$

where ε_1, ε_2, and ε_3 are dimensionless positive material constants. We also remark that for materials for which $\varepsilon_p = \varepsilon_m$, the dielectric tensor (3) reduces to (9) with $\varepsilon_1 = \varepsilon_2 = \varepsilon_p = \varepsilon_m$ and $\varepsilon_3 = \varepsilon_n$.

To model elastic contributions, we start from the elastic free energy density for an orthorhombic system presented in Stallinga and Vertogen (1994) and, as done in Vaupotič et al. (2014), for simplicity we do not include the higher order derivatives terms, i.e. the linear second-order terms of equation (26) in Stallinga and Vertogen (1994) (see also Trebin (1981) and Longa et al. (1998)).

Using $|\mathbf{p}| = 1$ and the assumption $\mathbf{n} = \mathbf{e}_3$, which implies (2) and $\mathbf{m} = \mathbf{n} \times \mathbf{p} = (-p_2, p_1, 0)$, this elastic density simplifies to the expression (see equation (A14) in Stallinga and Vertogen (1994)):

$$
\begin{aligned}
& k_1\,\mathbf{p}\cdot(\nabla\times\mathbf{p}) + k_2\,\mathbf{m}\cdot(\nabla\times\mathbf{m}) + \frac{1}{2}K_1(\nabla\cdot\mathbf{p})^2 + \frac{1}{2}K_2(\nabla\cdot\mathbf{m})^2 \\
& \quad + \frac{1}{2}K_4\left[\mathbf{p}\cdot(\nabla\times\mathbf{p})\right]^2 + \frac{1}{2}K_5\left[\mathbf{m}\cdot(\nabla\times\mathbf{m})\right]^2 + \frac{1}{2}K_7\left[\mathbf{n}\cdot(\nabla\times\mathbf{m})\right]^2 \\
& \quad + \frac{1}{2}K_{11}\left[\mathbf{n}\cdot(\nabla\times\mathbf{p})\right]^2 + K_{13}\left[\mathrm{Tr}(\nabla\mathbf{p})^2 - (\nabla\cdot\mathbf{p})^2\right] \\
& \quad + K_{14}\left[\mathrm{Tr}(\nabla\mathbf{m})^2 - (\nabla\cdot\mathbf{m})^2\right],
\end{aligned}
$$

where we also applied the following identity, which holds for any $\mathbf{u}\in\mathbf{H^1}(\mathbb{R}^\mathbf{3},\mathbb{R}^\mathbf{3})$ in the sense of distributions

$$
\nabla\cdot[(\mathbf{u}\cdot\nabla)\mathbf{u} - (\nabla\cdot\mathbf{u})\mathbf{u}] = \mathrm{Tr}(\nabla\mathbf{u})^2 - (\nabla\cdot\mathbf{u})^2.
$$

Substituting $\mathbf{m} = (-p_2, p_1, 0)$, we then have

$$
\begin{aligned}
f_e &= (k_1+k_2)\,\mathbf{p}\cdot(\nabla\times\mathbf{p}) + \frac{1}{2}(K_1+K_7)(\nabla\cdot\mathbf{p})^2 \\
&\quad + \frac{1}{2}(K_2+K_{11})\left[\mathbf{n}\cdot(\nabla\times\mathbf{p})\right]^2 + \frac{1}{2}(K_4+K_5)\left[\mathbf{p}\cdot(\nabla\times\mathbf{p})\right]^2 \\
&\quad + (K_{13}+K_{14})\left[\mathrm{Tr}(\nabla\mathbf{p})^2 - (\nabla\cdot\mathbf{p})^2\right].
\end{aligned}
\tag{10}
$$

We next add a linear term, which models dipolar divergence distortions and is needed because in bent-core molecules one distinguishes between the positive and negative directions of $\mathbf{P}$, see Coleman et al. (2003), Bailey et al. (2007), and Bauman and Phillips (2012):

$$
f_P = c'\nabla\cdot\mathbf{p} + c''\nabla\cdot\mathbf{P}. \tag{11}
$$

As a consequence of the divergence theorem, this term gives only a boundary contribution. Assuming $\mathbf{P} = P_0\,\mathbf{p}$ with P_0 constant, we have

$$
f_P = (c' + c''P_0)\nabla\cdot\mathbf{p} = c_P(P_0)\,\nabla\cdot\mathbf{p}.
$$

In conclusion, for P_0 constant, we arrive to the following phenomenological energy functional, together with (5):

$$
\begin{aligned}
&\int_{\Omega_t^L}\Bigg[k_T\,\mathbf{p}\cdot(\nabla\times\mathbf{p}) + \frac{1}{2}K_S\,(\nabla\cdot\mathbf{p})^2 + \frac{1}{2}K_B\left[\mathbf{n}\cdot(\nabla\times\mathbf{p})\right]^2 \\
&\quad + \frac{1}{2}K_T\left[\mathbf{p}\cdot(\nabla\times\mathbf{p})\right]^2 + \frac{1}{2}\,K_G\left[\mathrm{Tr}(\nabla\mathbf{p})^2 - (\nabla\cdot\mathbf{p})^2\right] \\
&\quad + c_P(P_0)\,\nabla\cdot\mathbf{p} - \mathbf{P}\cdot E_i - \mathbf{P}\cdot E_{ex}\Bigg] + \int_{\mathbb{R}^3}\frac{1}{2}\varepsilon_0\,\varepsilon^*_{\Omega_t^L}(\mathbf{p})\,E_i\cdot E_i,
\end{aligned}
\tag{12}
$$

where $k_T = k_1 + k_2$, $K_S = K_1 + K_7$, $K_B = K_2 + K_{11}$, $K_T = K_4 + K_5$, and $K_G = 2\,(K_{13} + K_{14})$.

We rewrite the K_G term using the identity: $\mathrm{Tr}(\nabla \mathbf{p})^2 = |\nabla \mathbf{p}|^2 - |\nabla \times \mathbf{p}|^2$, introduce the quantities

$$\mathrm{div}'\mathbf{p} = \partial_1 p_1 + \partial_2 p_2 \quad \text{and} \quad \mathrm{curl}'\mathbf{p} = \partial_1 p_2 - \partial_2 p_1,$$

and use (2) and $|\mathbf{p}| = 1$ to see that

$$\begin{aligned}&\nabla \cdot \mathbf{p} = \mathrm{div}'\mathbf{p}; \qquad \left[\mathbf{n} \cdot (\nabla \times \mathbf{p})\right]^2 = (\mathrm{curl}'\mathbf{p})^2,\\ &\mathbf{p} \cdot (\nabla \times \mathbf{p}) = (p_2\, \partial_3 p_1 - p_1\, \partial_3 p_2),\\ &-2\, p_1\, p_2\, \partial_3 p_1\, \partial_3 p_2 = p_1^2(\partial_3 p_1)^2 + p_2^2(\partial_3 p_2)^2,\end{aligned}$$

which gives

$$\begin{aligned}&[\mathbf{p} \cdot (\nabla \times \mathbf{p})]^2 = (\partial_3 p_1)^2 + (\partial_3 p_2)^2 = |\partial_3 \mathbf{p}|^2;\\ &|\nabla \times \mathbf{p}|^2 = |\partial_3 \mathbf{p}|^2 + (\mathrm{curl}'\mathbf{p})^2; \quad \mathrm{Tr}(\nabla \mathbf{p})^2 = |\nabla \mathbf{p}|^2 - |\partial_3 \mathbf{p}|^2 - (\mathrm{curl}'\mathbf{p})^2.\end{aligned}$$

We apply (5) to express E_i in terms of the electric potential:

$$\begin{aligned}\int_{\mathbb{R}^3} \varepsilon_0\, \varepsilon^*_{\Omega_t^L}(\mathbf{p})\, E_i \cdot E_i &= \int_{\mathbb{R}^3} \varepsilon_0\, \varepsilon^*_{\Omega_t^L}(\mathbf{p}) \nabla \Phi_t^L \cdot \nabla \Phi_t^L\\ &= \int_{\Omega_t^L} \mathbf{P} \cdot \nabla \Phi_t^L\, dx = -\int_{\Omega_t^L} \mathbf{P} \cdot E_i.\end{aligned}$$

Setting

$$\mathbf{p}^\perp = \mathbf{m} = (-p_2, p_1, 0), \tag{13}$$

our energy functional then becomes

$$\begin{aligned}\mathcal{E}(\mathbf{p}) = \int_{\Omega_t^L} \Big[&-k_T\, \mathbf{p}^\perp \cdot \partial_3 \mathbf{p} + \frac{1}{2}(K_S - K_G)\left(\mathrm{div}'\mathbf{p}\right)^2\\ &+ \frac{1}{2}(K_B - K_G)(\mathrm{curl}'\mathbf{p})^2 + \frac{1}{2}(K_T - K_G)|\partial_3 \mathbf{p}|^2 + \frac{1}{2} K_G\, |\nabla \mathbf{p}|^2\\ &+ c_p(P_0)\, \mathrm{div}'\mathbf{p} - P_0\, \mathbf{p} \cdot E_{ex} \Big] + \int_{\mathbb{R}^3} \frac{3}{2} \varepsilon_0\, \varepsilon^*_{\Omega_t^L}(\mathbf{p})\, \nabla \Phi_t^L \cdot \nabla \Phi_t^L,\end{aligned} \tag{14}$$

with Gauss's law

$$\varepsilon_0\, \nabla \cdot \left(\varepsilon^*_{\Omega_t^L}(\mathbf{p})\, \nabla \Phi_t^L\right) = P_0\, \nabla \cdot (\mathbf{p} \chi_{\Omega_t^L}) \quad \text{in } \mathbb{R}^3. \tag{15}$$

We look for minimizers $\mathbf{p}$ of (14) in $H^1(\Omega_t^L, S^2)$, where recall that for $\mathbf{p} \in H^1(\Omega_t^L, S^2)$, the function $\mathbf{p}\chi_{\Omega_t^L}$ is to be interpreted as $\mathbf{p}\, \chi_{\Omega_t^L} = \mathbf{p}$ in Ω_t^L and zero elsewhere.

By elliptic regularity theory (15) has a solution $\Phi_t^L \in L^6(\mathbb{R}^3)$, with $\nabla \Phi_t^L \in L^2(\mathbb{R}^3, \mathbb{R}^3)$ (see Sect. 3.1 below). And, existence of minimizers is straightforward under our assumptions, provided that

$$
\begin{aligned}
&K_S \geq 0; \qquad K_B \geq 0; \qquad K_T \geq 0; \qquad K_G > 0;\\
&K_S - K_G \geq 0; \qquad K_B - K_G \geq 0; \qquad K_T - K_G \geq 0,
\end{aligned} \tag{16}
$$

with no sign restriction on k_T and c_p.

2.1 Dimensionless Energy

To understand the role of the relative size of the cell thickness t and the cell size L, we rescale length by L, the electric potential by $\frac{L\,P_0}{\varepsilon_0}$, and the energy by $\frac{P_0^2\,L^3}{\varepsilon_0}$, and work with the dimensionless quantities:

$$
\begin{aligned}
&\widehat{\mathbf{x}} = \frac{\mathbf{x}}{L}, \quad h = \frac{t}{L}; \quad \widehat{\Phi}_h = \frac{\varepsilon_0}{L\,P_0}\,\Phi_h^1; \quad \Omega_h = (0,1)^2 \times (0,h)\,,\\
&\sigma = \frac{L^2\,P_0\,|E_{ex}|}{K_G}, \quad k_T^* = \frac{k_T}{K_G}, \quad K_S^* = \frac{K_S - K_G}{K_G},\\
&K_B^* = \frac{K_B - K_G}{K_G}, \quad K_T^* = \frac{K_T - K_G}{K_G}, \quad c_p^* = \frac{c_p(P_0)L}{K_G}.
\end{aligned}
$$

Recalling that we are assuming E_{ex} constant, given $\mathbf{e}$, a unit vector parallel to the direction of E_{ex}, we write $E_{ex} = \sigma_s\,|E_{ex}|\,\mathbf{e}$, where $\sigma_s = \mathrm{sign}(E_{ex})$, and dropping the hat in the rescaled quantities, for $\mathbf{p}_h \in H^1(\Omega_h, S^2)$ we arrive at the following dimensionless energy:

$$
\begin{aligned}
\mathcal{E}_h(\mathbf{p}_h) = \frac{\varepsilon_0\,K_G}{2P_0^2L^2}\int_{\Omega_h}\Big[&-2k_T^*\,\mathbf{p}_h^{\perp}\cdot\partial_3\mathbf{p}_h + K_S^*\,\big(\mathrm{div}'\mathbf{p}_h\big)^2 + K_B^*\,(\mathrm{curl}'\mathbf{p}_h)^2\\
&+ K_T^*\,|\partial_3\mathbf{p}_h|^2 + |\nabla\mathbf{p}_h|^2 + 2\,c_p^*\,\mathrm{div}'\mathbf{p}_h - 2\,\sigma_s\,\sigma\,\mathbf{p}_h\cdot\mathbf{e}\Big]\\
&+ \int_{\mathbb{R}^3}\frac{3}{2}\varepsilon_h^*(\mathbf{p}_h)\,\nabla\Phi_h\cdot\nabla\Phi_h,
\end{aligned} \tag{17}
$$

augmented by the Gauss's law

$$
\nabla\cdot\big(\varepsilon_h^*(\mathbf{p}_h)\,\nabla\Phi_h\big) = \nabla\cdot(\mathbf{p}_h\,\chi_{\Omega_h}) \quad \text{in } \mathbb{R}^3, \tag{18}
$$

where $\varepsilon_h^*(\mathbf{p}_h) := \varepsilon_{\Omega_h}^*(\mathbf{p}_h)$. Note that for $\varepsilon_h^*(\mathbf{p}_h)$ we still have the estimates in (7), this is a property that we will use in a fundamental way.

3 Preliminary Results

We follow the idea of Kohn and Slastikov (2005) and study a rescaled small thickness limit of (17) for the case of a constant applied field E_{ex} parallel to the y direction. Using the properties of the fundamental solutions of the uniformly elliptic equation (18), inferred from some classical Littman et al. (1963) and recent Mourgoglou (2019) work, we show that under some technical assumptions on the dielectric tensor and domain thickness the electric potential term gives rise to boundary terms. These boundary terms, in the one-dimensional setup, agree with the ones proposed in the work of Gornik and coauthors (Gornik et al. 2014; Gornik and Vaupotič 2014). We proceed by obtaining some preliminary estimates.

3.1 Fundamental Solutions

The dimensionless Gauss's law (18) is a second-order elliptic equation in divergence form of the type

$$\sum_{i,j=1}^{3} \partial_i \left(a_{ij}(\mathbf{x})\, \partial_j\, u(\mathbf{x})\right) = \sum_{i=1}^{3} \partial_i\, g_i(\mathbf{x}) \quad \text{for } \mathbf{x} \in \mathbb{R}^3, \tag{19}$$

where $\mathbf{g} = (g_1, g_2, g_3) \in L^p(\mathbb{R}^3, \mathbb{R}^3)$ for all $p \geq 1$, and $a_{ij}(\mathbf{x}) \in L^\infty(\mathbb{R}^3)$ with

$$\sum_{i,j=1}^{3} a_{ij}(\mathbf{x}) x_i\, x_j \geq \underline{\epsilon}\, |\mathbf{x}|^2; \qquad \sum_{i,j=1}^{3} a_{ij}(\mathbf{x}) x_i\, y_j \leq \overline{\epsilon}\, |\mathbf{x}|\, |\mathbf{y}|. \tag{20}$$

Consider the space $Y^{1,2}(\mathbb{R}^3) = \left\{u \in L^6(\mathbb{R}^3) : \nabla u \in L^2(\mathbb{R}^3, \mathbb{R}^3)\right\}$. For general properties of $Y^{1,2}(\mathbb{R}^3)$ we refer to Malý and Ziemer Malý and Ziemer (1997). In particular, $Y^{1,2}(\mathbb{R}^3)$ is endowed with the norm

$$||u||_Y := ||u||_{L^6} + ||\nabla u||_{L^2}, \tag{21}$$

and $Y_0^{1,2}(\mathbb{R}^3) = Y^{1,2}(\mathbb{R}^3)$, where $Y_0^{1,2}(\mathbb{R}^3)$ is the closure of $C_c^\infty(\mathbb{R}^3)$ in $Y^{1,2}(\mathbb{R}^3)$. Moreover, for $u \in Y^{1,2}(\mathbb{R}^3)$, it holds

$$||u||_{L^6} \leq C||\nabla u||_{L^2}, \tag{22}$$

for some constant $C = C(n)$ (see Malý and Ziemer (1997) Lemma 1.76 pg. 46).

Green's functions for second-order elliptic equation with bounded measurable coefficients in divergence form were well studied by Littman, Stampacchia, and Weinberger in Littman et al. (1963) and later by Grüter and Widman in Grüter and Widman (1982). More recently, Hofmann and Kim in Hofmann and Kim (2007) studied Green's matrices of strongly elliptic systems under the assumption that solutions of the elliptic system satisfy De Giorgi-Nash type local Hölder continuity estimates, which is satisfied for the scalar case (see Gilbarg and Trudinger (1998), also mentioned in Kang and Kim (2010)). More detailed analysis for elliptic equations with lower order terms can be found in Mourgoglou (2019).

Recall that we denote by L_c^∞ the family of L^∞ functions with compact support.

Lemma 3.1 *Let $A = (a_{ij})$ with $a_{ij} \in L^\infty(\mathbb{R}^3)$ $(i, j = 1..3)$ verify (20). Assume $\boldsymbol{g} \in L^\infty_c(\mathbb{R}^3, \mathbb{R}^3)$, then a fundamental solution $K(\mathbf{x}, \mathbf{y}; A)$ of the operator*

$$L(u) = -\sum_{i,j=1}^{3} \partial_i \left(a_{ij}(\mathbf{x})\, \partial_j\, u(\mathbf{x})\right)$$

exists, with $K(\cdot, \mathbf{y}; A) \in W^{1,1}_{loc}(\mathbb{R}^3)$. Additionally,

$$\boldsymbol{u}(\mathbf{x}) = \int_{\mathbb{R}^3} \mathbf{g}(\boldsymbol{y}) \cdot \nabla_{\mathbf{y}} K(\mathbf{x}, \mathbf{y}; A)\, d\mathbf{y} \tag{23}$$

is the unique solution in $Y^{1,2}(\mathbb{R}^3)$ of $L(u) = -\nabla \cdot \boldsymbol{g}$. Moreover, $K(\mathbf{x}, \mathbf{y}; A) = K(\mathbf{y}, \mathbf{x}; A)$ a.e., and for some constant $C_0 > 0$, which depends only on the constants $\underline{\epsilon}$ and $\overline{\epsilon}$, it holds

$$C_0^{-1}\, |\mathbf{x} - \mathbf{y}|^{-1} \leq K(\mathbf{x}, \mathbf{y}; A) \leq C_0\, |\mathbf{x} - \mathbf{y}|^{-1} \tag{24}$$

for a.e. $\mathbf{x} \in \mathbb{R}^3 \setminus \{\mathbf{y}\}$.

Proof The existence and the properties of $K(\mathbf{x}, \mathbf{y}; A)$, as well as the representation formula (23) follow for example from Theorem 6.1 in Mourgoglou (2019). While for the symmetry property, and the bound (24) we refer to Littman et al. (1963). In particular, the argument that leads to (7.9) pg 67 in Littman et al. (1963) can be applied to obtain the global bound, the symmetry property, and Hölder continuity in $\mathbb{R}^3 \setminus \{\mathbf{y}\}$. See also Theorem 3.1 for the symmetry property and the global estimate, and Theorem 3.2 in Hofmann and Kim (2007) for the representation formula, as well as part (3) of Theorem 6.1 and Lemma 6.4 in Mourgoglou (2019). □

3.2 Averaging Along the Thickness

Setting $\mathbf{x} = (x_1, x_2, x_3) \in \Omega_h$, for a given $\mathbf{p}_h(\mathbf{x}) \equiv \mathbf{p}_h(x_1, x_2, x_3) \in H^1(\Omega_h, S^2)$ and using the notation $\overline{\mathbf{p}}_h(x_1, x_2) = \frac{1}{h}\int_0^h \mathbf{p}_h(x_1, x_2, x_3)\, dx_3$, we consider the solution $\overline{\Phi}_h$ of

$$\nabla \cdot \left(\varepsilon_h^*(\mathbf{p}_h)\, \nabla\overline{\Phi}_h\right) = \nabla \cdot (\overline{\mathbf{p}}_h \chi_{\Omega_h}) \quad \text{in } \mathbb{R}^3, \tag{25}$$

where recall that $\varepsilon_h^*(\mathbf{p}_h) := \varepsilon^*_{\Omega_h}(\mathbf{p}_h)$ and $\varepsilon^*_{\Omega_h}(\mathbf{p}_h)$ is defined via (3) and (6). It is important to stress that while $\overline{\mathbf{p}}_h$ does not depend on x_3, the right-hand side and the coefficients of (25) do, and therefore the solution does depend on x_3. Note also that we are employing $\varepsilon_h^*(\mathbf{p}_h)$ rather than $\varepsilon_h^*(\overline{\mathbf{p}}_h)$, and that (25) is of the type (19) as well.

We start by proving a result analogous to Lemma 3 in Kohn and Slastikov (2005).

Lemma 3.2 *Let $\mathbf{p}_h \in H^1(\Omega_h, S^2)$ and Φ_h and $\overline{\Phi}_h$ be the solutions of (18) and (25), respectively. There is a universal constant C such that*

$$\left| \int_{\mathbb{R}^3} \varepsilon_h^*(\mathbf{p}_h) \nabla\Phi_h \cdot \nabla\Phi_h - \int_{\mathbb{R}^3} \varepsilon_h^*(\mathbf{p}_h) \nabla\overline{\Phi}_h \cdot \nabla\overline{\Phi}_h \right| \leq C \sqrt{\frac{\overline{\epsilon}}{\underline{\epsilon}^3}} \left(h^2 + \int_{\Omega_1} (\partial_3\, \widetilde{\mathbf{p}}_h)^2\right). \tag{26}$$

Proof We simply write ε^* for $\varepsilon_h^*(\mathbf{p}_h)$.

By definition of weak solutions in $Y^{1,2}(\mathbb{R}^3)$, for any $\phi \in C_c^\infty(\mathbb{R}^3)$, we have

$$\int_{\mathbb{R}^3} \varepsilon^*(\nabla\Phi_h - \nabla\overline{\Phi}_h)\cdot\nabla\phi = \int_{\mathbb{R}^3} \left(\mathbf{p}_h\chi_{\Omega_h} - \overline{\mathbf{p}}_h\chi_{\Omega_h}\right)\cdot\nabla\phi,$$

and taking a sequence $\phi_n \in C_c^\infty(\mathbb{R}^3)$ converging to $\Phi_h - \overline{\Phi}_h$ in $Y^{1,2}(\mathbb{R}^3)$, we conclude

$$\begin{aligned}\int_{\mathbb{R}^3} \varepsilon^*(\nabla\Phi_h - \nabla\overline{\Phi}_h)\cdot(\nabla\Phi_h - \nabla\overline{\Phi}_h) &= \int_{\mathbb{R}^3} \left(\mathbf{p}_h\chi_{\Omega_h} - \overline{\mathbf{p}}_h\chi_{\Omega_h}\right)\cdot\nabla(\Phi_h - \overline{\Phi}_h)\\ &\le \|\mathbf{p}_h - \overline{\mathbf{p}}_h\|_{L^2(\Omega_h)}\|\nabla\Phi_h - \nabla\overline{\Phi}_h\|_{L^2(\mathbb{R}^3)}.\end{aligned} \tag{27}$$

Using this together with the uniform ellipticity (4), we obtain

$$\|\nabla\Phi_h - \nabla\overline{\Phi}_h\|_{L^2(\mathbb{R}^3)} \le \frac{1}{\varepsilon_-}\|\mathbf{p}_h - \overline{\mathbf{p}}_h\|_{L^2(\Omega_h)}. \tag{28}$$

Since ε^* is positive definite, its square root is uniquely defined and denoted by B. Then we have

$$\begin{aligned}&\left|\int_{\mathbb{R}^3} \varepsilon^*\nabla\Phi_h\cdot\nabla\Phi_h - \varepsilon^*\nabla\overline{\Phi}_h\cdot\nabla\overline{\Phi}_h\right|\\ &= \left|\int_{\mathbb{R}^3} |B\nabla\Phi_h|^2 - \int_{\mathbb{R}^3} |B\nabla\overline{\Phi}_h|^2\right|\\ &= \left|\|B\nabla\Phi_h\|_{L^2(\mathbb{R}^3)} - \|B\nabla\overline{\Phi}_h\|_{L^2(\mathbb{R}^3)}\right|\cdot\left|\|B\nabla\Phi_h\|_{L^2(\mathbb{R}^3)} + \|B\nabla\overline{\Phi}\|_{L^2(\mathbb{R}^3)}\right|\\ &=: I_1\, I_2.\end{aligned}$$

By (27) and (28), we find

$$\begin{aligned}I_1^2 &\le \|B\nabla\Phi_h - B\nabla\overline{\Phi}_h\|^2_{L^2(\mathbb{R}^3)} = \int_{\mathbb{R}^3} \varepsilon^*\left(\nabla\Phi_h - \nabla\overline{\Phi}_h\right)\cdot\left(\nabla\Phi_h - \nabla\overline{\Phi}_h\right)\\ &\le \|\mathbf{p}_h - \overline{\mathbf{p}}_h\|_{L^2(\Omega_h)}\|\nabla\Phi_h - \nabla\overline{\Phi}_h\|_{L^2(\mathbb{R}^3)}\\ &\le \|\mathbf{p}_h - \overline{\mathbf{p}}_h\|_{L^2(\Omega_h)}\frac{1}{\varepsilon_-}\|\mathbf{p}_h - \overline{\mathbf{p}}_h\|_{L^2(\Omega_h)}\end{aligned}$$

and then applying the Poincaré inequality yields

$$I_1 \le \frac{1}{\sqrt{\varepsilon_-}}\|\mathbf{p}_h - \overline{\mathbf{p}}_h\|_{L^2(\Omega_h)} \le \frac{Ch}{\sqrt{\varepsilon_-}}\left\|\frac{\partial\mathbf{p}_h}{\partial z}\right\|_{L^2(\Omega_h)}.$$

Now we estimate I_2. Applying the same proof for (28) on $\nabla\Phi_h$,

$$\|B\nabla\Phi_h\|^2_{L^2(\mathbb{R}^3)} = \int_{\mathbb{R}^3} \varepsilon^* \nabla\Phi_h \cdot \nabla\Phi_h \le \varepsilon_+ \|\nabla\Phi_h\|^2_{L^2(\mathbb{R}^3)}$$
$$\le \frac{\varepsilon_+}{\varepsilon_-^2}\|\mathbf{p}_h\|^2_{L^2(\Omega_h)} = \frac{Ch\varepsilon_+}{\varepsilon_-^2}.$$

Similarly we obtain the estimate for $B\nabla\overline{\Phi}_h$. These two inequalities give

$$I_2 \le C\sqrt{h}\frac{\sqrt{\varepsilon_+}}{\varepsilon_-}.$$

Combining these estimates for I_1 and I_2, we have the desired inequality:

$$\begin{aligned}\left|\int_{\mathbb{R}^3} \varepsilon^*\nabla\Phi_h \cdot \nabla\Phi_h - \varepsilon^*\nabla\overline{\Phi}_h \cdot \nabla\overline{\Phi}_h\right| &\le \frac{Ch\sqrt{h\varepsilon_+}}{\varepsilon_-\sqrt{\varepsilon_-}}\left\|\frac{\partial \mathbf{p}_h}{\partial z}\right\|_{L^2(\Omega_h)} \\ &\le \frac{C\sqrt{\varepsilon_+}h}{\varepsilon_-^{3/2}}\left\|\frac{\partial \widetilde{\mathbf{p}}_h}{\partial z}\right\|_{L^2(\Omega_1)} \\ &\le C\frac{\sqrt{\varepsilon_+}}{\varepsilon_-^{3/2}}\left(h^2 + \int_{\Omega_1}\left|\frac{\partial \widetilde{\mathbf{p}}_h}{\partial z}\right|^2\right).\end{aligned}$$

□

3.3 The Electric Potential Term

As in Kohn and Slastikov (2005), because of (26), we focus our attention on the term $\int_{\mathbb{R}^3} \varepsilon_h^*(\mathbf{p}_h)\, \nabla\overline{\Phi}_h \cdot \nabla\overline{\Phi}_h$.

We fix $\mathbf{p}_h \in H^1(\Omega_h, S^2)$, and denote by $K_h(\mathbf{x}, \mathbf{y}; \mathbf{p}_h)$ the fundamental solution of (25). Using Lemma 3.1 we see that

$$\begin{aligned}\overline{\Phi}_h(\mathbf{x}) &= \int_{\mathbb{R}^3} \overline{\mathbf{p}}_\mathbf{h}\, \chi_{\Omega_h} \cdot \nabla_\mathbf{y} K_h(\mathbf{x}, \mathbf{y}; \mathbf{p}_h)\, d\mathbf{y} \\ &= -\int_{\Omega_h} \nabla \cdot \overline{\mathbf{p}}_h(\mathbf{y})\, K_h(\mathbf{x}, \mathbf{y}; \mathbf{p}_h)\, d\mathbf{y} + \int_{\partial\Omega_h} K_h(\mathbf{x}, \mathbf{y}; \mathbf{p}_h)\, \left(\overline{\mathbf{p}}_h \cdot \nu\right)(\mathbf{y})\, d\sigma_\mathbf{y} \\ &= -\int_{\Omega_h} \mathrm{div}'\, \overline{\mathbf{p}}_h(\mathbf{y})\, K_h(\mathbf{x}, \mathbf{y}; \mathbf{p}_h)\, d\mathbf{y} + \int_{\partial\Omega_h} K_h(\mathbf{x}, \mathbf{y}; \mathbf{p}_h)\, \left(\overline{\mathbf{p}}_h \cdot \nu\right)(\mathbf{y})\, d\sigma_\mathbf{y}.\end{aligned} \tag{29}$$

One should notice that because of the global bound (24) the above integrals are well-defined. By definition of weak solution of (18) in $Y^{1,2}(\mathbb{R}^3)$, for any $\phi \in C_c^\infty(\mathbb{R}^3)$, we have

$$\int_{\mathbb{R}^3} \varepsilon_h^*(\mathbf{p}_h)\, \nabla\overline{\Phi}_h \cdot \nabla\phi = \int_{\mathbb{R}^3} \overline{\mathbf{p}}_h(\mathbf{x})\chi_{\Omega_h}(\mathbf{x}) \cdot \nabla\phi(\mathbf{x})\, d\mathbf{x}.$$

Hence,

$$\int_{\mathbb{R}^3} \varepsilon_h^*(\mathbf{p}_h)\, \nabla\overline{\Phi}_h \cdot \nabla\phi = -\int_{\Omega_h} \nabla\cdot\overline{\mathbf{p}}_h\, \phi + \int_{\partial\Omega_h} (\overline{\mathbf{p}}_h\cdot\nu)\,\phi,$$

and taking a sequence $\phi_n \in C_c^\infty(\mathbb{R}^3)$ converging to $\overline{\Phi}_h$ in $Y^{1,2}(\mathbb{R}^3)$, we gather

$$\int_{\mathbb{R}^3} \varepsilon_h^*(\mathbf{p}_h)\, \nabla\overline{\Phi}_h \cdot \nabla\overline{\Phi}_h = -\int_{\Omega_h} \overline{\Phi}_h\, \mathrm{div}'\overline{\mathbf{p}}_h + \int_{\partial\Omega_h} \overline{\Phi}_h(\mathbf{x})\, (\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\, d\sigma_{\mathbf{x}}, \tag{30}$$

Using (29) in (30), we find

$$\begin{aligned}\int_{\mathbb{R}^3} \varepsilon_h^*(\mathbf{p}_h)\, \nabla\overline{\Phi}_h \cdot \nabla\overline{\Phi}_h = &\int_{\Omega_h}\int_{\Omega_h} \mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y})\; \mathrm{div}'\overline{\mathbf{p}}_h(\mathbf{x})\, K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\, d\mathbf{y}\, d\mathbf{x}\\ &-\int_{\Omega_h}\int_{\partial\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\, \big(\overline{\mathbf{p}}_h\cdot\nu\big)(\mathbf{y})\, \mathrm{div}'\overline{\mathbf{p}}_h(\mathbf{x})\, d\sigma_{\mathbf{y}}\, d\mathbf{x}\\ &-\int_{\partial\Omega_h}\int_{\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\, \mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y})\, (\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\, d\mathbf{y}\, d\sigma_{\mathbf{x}}\\ &+\int_{\partial\Omega_h}\int_{\partial\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\, \big(\overline{\mathbf{p}}_h\cdot\nu\big)(\mathbf{y})\, (\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\, d\sigma_{\mathbf{y}}\, d\sigma_{\mathbf{x}}\end{aligned}$$

and by the symmetry of the fundamental solution we conclude

$$\begin{aligned}\int_{\mathbb{R}^3} \varepsilon_h^*(\mathbf{p}_h)\, \nabla\overline{\Phi}_h \cdot \nabla\overline{\Phi}_h = &\int_{\Omega_h}\int_{\Omega_h} \mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y})\; \mathrm{div}'\overline{\mathbf{p}}_h(\mathbf{x})\, K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\, d\mathbf{y}\, d\mathbf{x}\\ &-2\int_{\partial\Omega_h}\int_{\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\, \mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y})\, (\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\, d\mathbf{y}\, d\sigma_{\mathbf{x}}\\ &+\int_{\partial\Omega_h}\int_{\partial\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\, \big(\overline{\mathbf{p}}_h\cdot\nu\big)(\mathbf{y})\, (\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\, d\sigma_{\mathbf{y}}\, d\sigma_{\mathbf{x}}.\end{aligned} \tag{31}$$

One should remark that the argument leading to (7.9) pg 67 in Littman et al. (1963) can be applied to obtain Hölder continuity in $\mathbb{R}^3 \setminus \{\mathbf{y}\}$ of the fundamental solution $K_h(\cdot,\mathbf{y};\mathbf{p}_h)$, see also Sect. 3.6 in Hofmann and Kim (2007). We estimate each integral in (31) separately. From the point of view of this work, the third integral is the one of most interest, as it gives rise to boundary terms in the limit.

Lemma 3.3 *Let $\mathbf{p}_h \in H^1(\Omega_h, S^2)$. Under our assumptions, we have that*

$$\left|\int_{\Omega_h}\int_{\Omega_h} div'\,\overline{\mathbf{p}}_h(\mathbf{y})\; div'\overline{\mathbf{p}}_h(\mathbf{x})\, K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\, d\mathbf{y}\, d\mathbf{x}\right| \le C\, h^2\, ||div'\widetilde{\mathbf{p}}_h||^2_{L^2(\Omega_1)}. \tag{32}$$

Proof We introduce the compactly supported kernel

$$k(x_1,x_2)=\frac{1}{\sqrt{x_1^2+x_2^2}}\,\chi_{\left\{\sqrt{x_1^2+x_2^2}\le 2\right\}},$$

and define

$$\phi(x_1,x_2)=\int_{(0,1)^2}\left|\mathrm{div}'\overline{\mathbf{p}}_h(y_1,y_2))\right|k(x_1-y_1,x_2-y_2)\,dy_1dy_2.$$

By Young's inequality, since $k\in L^1(\mathbb{R}^2)$, we then have $\phi\in L^2(\mathbb{R}^2)$ and $\|\phi\|_{L^2(\mathbb{R}^2)}\le \|k\|_{L^1(\mathbb{R}^2)}\|\mathrm{div}'\overline{\mathbf{p}}_h\|_{L^2((0,1)^2)}$.

As a consequence of (24), we can use a similar approach to that in Kohn and Slastikov (2005) to get, using $\mathbf{x}'=(x_1,x_2)$, $\mathbf{y}'=(y_1,y_2)$, and $\omega=(0,1)^2$,

$$\begin{aligned}
&\left|\int_{\Omega_h}\int_{\Omega_h}\mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y})\;\mathrm{div}'\overline{\mathbf{p}}_h(\mathbf{x})\,K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\,d\mathbf{y}\,d\mathbf{x}\right|\\
&\quad=\left|\int_\omega\int_\omega\mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y}')\;\mathrm{div}'\overline{\mathbf{p}}_h(\mathbf{x}')\int_0^h\int_0^h K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\,dx_3\,dy_3\,d\mathbf{y}'\,d\mathbf{x}'\right|\\
&\quad\le C\int_\omega\int_\omega|\mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y}')|\;|\mathrm{div}'\overline{\mathbf{p}}_h(\mathbf{x}')|\int_0^h\int_0^h|\mathbf{x}-\mathbf{y}|^{-1}\,dx_3\,dy_3\,d\mathbf{y}'\,d\mathbf{x}'\\
&\quad\le C\,h^2\int_\omega\int_\omega\frac{|\mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y}')|\;|\mathrm{div}'\overline{\mathbf{p}}_h(\mathbf{x}')|}{\left[(x_1-y_1)^2+(x_2-y_2)^2\right]^{1/2}}\,d\mathbf{y}'\,d\mathbf{x}',
\end{aligned}$$

by Hölder inequality we arrive to the wanted bound:

$$\begin{aligned}
&\left|\int_{\Omega_h}\int_{\Omega_h}\mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y})\;\mathrm{div}'\overline{\mathbf{p}}_h(\mathbf{x})\,K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\,d\mathbf{y}\,d\mathbf{x}\right|\\
&\quad\le C\,h^2\int_{(0,1)^2}|\mathrm{div}'\overline{\mathbf{p}}_h(x_1,x_2)|\phi(x_1,x_2)\,dx_1\,dx_2\\
&\quad\le C\,h^2\,\|\mathrm{div}'\overline{\mathbf{p}}_h\|_{L^2((0,1)^2)}||\phi||_{L^2((0,1)^2)}\\
&\quad\le C\,h^2\,||\mathrm{div}'\overline{\mathbf{p}}_h||_{L^2((0,1)^2)}\;||\mathrm{div}'\overline{\mathbf{p}}_h||_{L^2((0,1)^2)}\le C\,h^2\,||\mathrm{div}'\widetilde{\mathbf{p}}_h||^2_{L^2(\Omega_1)}.
\end{aligned}$$

□

The difficulty in dealing with the second term in (31) stems from the fact that the boundary of the domain is not smooth and for a Lipschitz domain the trace operator $H^{1/2}(\Omega)\to L^2(\partial\Omega)$ does not exist (see Corollary 2.13, p. 331, in Mikhailov (2011)). However, the bound (24) allows us to control this term using a Riesz potential and applying the trace embedding theorem for $n=2$ and $p=\frac{4}{3}$.

Lemma 3.4 *Let $\mathbf{p}_h \in H^1(\Omega_h, S^2)$. Under our assumptions, it holds*

$$\left|\int_{\partial\Omega_h}\int_{\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\, div'\,\overline{\mathbf{p}}_h(\mathbf{y})\,(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\,d\mathbf{y}\,d\sigma_{\mathbf{x}}\right| \leq C\,h^2\left(1+||\,div'\widetilde{\mathbf{p}}_h\,||^2_{L^2(\Omega_1)}\right). \tag{33}$$

Proof Since $|(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})| \leq 1$, we can simplify our expression to

$$\left|\int_{\partial\Omega_h}\int_{\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\,\mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y})\,(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\,d\mathbf{y}\,d\sigma_{\mathbf{x}}\right| \leq C\int_{\partial\Omega_h}\int_{\Omega_h}|K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)|\,|\mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y})|\,d\mathbf{y}\,d\sigma_{\mathbf{x}}.$$

And, as in Lemma 3.3, using (24) and the Riesz potential, $0<\gamma<n$:

$$I_\gamma(f)(z) = c(\gamma,n)\int_{\mathbb{R}^n}\frac{f(w)}{|z-w|^{n-\gamma}}\,dw,\quad z\in\mathbb{R}^n,$$

with $n=2$, $\gamma=1$, and $f=|\mathrm{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}|$, we obtain

$$\left|\int_{\partial\Omega_h}\int_{\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\,\mathrm{div}'\,\overline{\mathbf{p}}_h(\mathbf{y})\,(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\,d\mathbf{y}\,d\sigma_{\mathbf{x}}\right| \leq C\,h^2\int_{\partial(0,1)^2} I_1\left(\left|\mathrm{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\right)\,d\sigma_{x_1,x_2}. \tag{34}$$

By Theorem 1.97 pg. 58 in Malý and Ziemer Malý and Ziemer (1997), we know that if $1<p<n$ and $f\in L^p(\mathbb{R}^n)$, then $I_1(f)\in Y^{1,p}(\mathbb{R}^n)$, and there is a constant $C_0=C_0(n,p)$, such that

$$C_0^{-1}\,||f||_{L^p} \leq ||I_1 f||_{Y^{1,p}} \leq C_0\,||f||_{L^p}, \tag{35}$$

where

$$||f||_{Y^{1,p}} := ||f||_{L^{p^*}} + ||\nabla f||_{L^p},\qquad p^* = \frac{np}{n-p}.$$

Applying, this result for $f=\left|\mathrm{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|$, $n=2$, and $p=4/3$, which gives $p^*=4$, we gather that $I_1\left(\left|\mathrm{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\right)\in W^{1,4/3}((0,1)^2)$, and by (35),

$$||I_1\left(\left|\mathrm{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\right)||_{W^{1,4/3}((0,1)^2)} \leq C\,\left|\left|\,\left|\mathrm{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\,\right|\right|_{L^{4/3}((0,1)^2)}. \tag{36}$$

A classical theorem for Lipschitz domains by Gagliardo (1957) then implies that $I_1\left(\left|\mathrm{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\right)\in L^{4/3}(\partial(0,1)^2)$, and

$$||I_1\left(\left|\mathrm{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\right)||_{L^{4/3}(\partial(0,1)^2)} \leq C_1\,||I_1\left(\left|\mathrm{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\right)||_{W^{1,4/3}((0,1)^2)},$$

which in turn, in conjunction with (36) and Hölder's inequality, gives

$$
\begin{aligned}
&||I_1\left(\left|\operatorname{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\right)||_{L^1(\partial(0,1)^2)} \le C\,||I_1\left(\left|\operatorname{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\right)||_{L^{4/3}(\partial(0,1)^2)}\\
&\quad\le\; C\;\left|\left|\,\left|\operatorname{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\,\right|\right|_{L^{4/3}((0,1)^2)} \le\; C\;\left|\left|\,\left|\operatorname{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\,\right|\right|_{L^{2}((0,1)^2)}.
\end{aligned}
$$

Since $I_1\left(\left|\operatorname{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\right)\,|\ge 0$, this and (34), imply

$$
\begin{aligned}
&\left|\int_{\partial\Omega_h}\int_{\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\,\operatorname{div}'\,\overline{\mathbf{p}}_h(\mathbf{y})\,(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\,d\mathbf{y}\,d\sigma_{\mathbf{x}}\right|\\
&\quad\le C\,h^2\;\;\left|\left|\,\left|\operatorname{div}'\overline{\mathbf{p}}_h\,\chi_{(0,1)^2}\right|\,\right|\right|_{L^{2}((0,1)^2)},
\end{aligned}
$$

and, our claim follows from (1), and the inequality $b\,a \le \frac{1}{2}(b^2+a^2)$, with $b=1$. □

To deal with the last term in (31) we follow a similar approach as the one in Kohn and Slastikov (2005), and we divide the integral into two parts: The first part is bounded in Lemma 3.5, and the second is considered in the next sections.

Since our domain has limited regularity having only a Lipschitz boundary, we cannot directly apply the method of proof of Kohn and Slastikov (2005), where the smoothness of the normal vector to the boundary is used in a fundamental way. In our case we need to keep track of the different parts of the boundary.

We denote by Γ_i, $i=1...4$, the four open sides of the $\partial(0,1)^2$:

$$
\begin{aligned}
\Gamma_1 &= \left\{(x_1,0)\in\mathbb{R}^2,\ 0<x_1<1\right\}; \qquad \Gamma_2 = \left\{(1,x_2)\in\mathbb{R}^2,\ 0<x_2<1\right\}\\
\Gamma_3 &= \left\{(x_1,1)\in\mathbb{R}^2,\ 0<x_1<1\right\}; \qquad \Gamma_4 = \left\{(0,x_2)\in\mathbb{R}^2,\ 0<x_2<1\right\}.
\end{aligned}
$$

Lemma 3.5 *Let $\mathbf{p}_h\in H^1(\Omega_h,S^2)$. Under our assumptions, we have that*

$$
\begin{aligned}
&\left|\int_{\partial\Omega_h}\int_{\partial\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\,\left[\left(\overline{\mathbf{p}}_h\cdot\nu\right)(\mathbf{y})-(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\right]\right.\\
&\qquad\qquad\left.(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\,d\sigma_{\mathbf{y}}\,d\sigma_{\mathbf{x}}\right| \le C\,h^2\left(||\overline{\mathbf{p}}_h||_{H^1((0,1)^2)}+1\right).
\end{aligned}
$$

Proof On the parts of $\partial\Omega_h$ with $x_3=0$, and $x_3=h$, the normal ν to $\partial\Omega_h$ is parallel to the x_3-axis, so that in there we have $(\overline{\mathbf{p}}_h\cdot\nu)(x_1,x_2,0)=(\overline{\mathbf{p}}_h\cdot\nu)(x_1,x_2,h)=0$, as $p_3=0$. Additionally, on the rest of $\partial\Omega_h$ the normal does not depend on x_3. Hence, on $\partial\Omega_h$ the function $(\overline{\mathbf{p}}_h\cdot\nu)$ does not depend on x_3, that is $(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})=(\overline{\mathbf{p}}_h\cdot\nu)(x_1,x_2)$.

Using $|(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})|\le 1$ and (24), we then arrive to

$$
\begin{aligned}
&\left|\int_{\partial\Omega_h}\int_{\partial\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\,\left[\left(\overline{\mathbf{p}}_h\cdot\nu\right)(\mathbf{y})-(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\right](\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})\,d\sigma_{\mathbf{y}}\,d\sigma_{\mathbf{x}}\right|\\
&\quad\le C\,h^2\int_{\partial(0,1)^2}\int_{\partial(0,1)^2}\frac{\left|\left(\overline{\mathbf{p}}_h\cdot\nu\right)(y_1,y_2)-(\overline{\mathbf{p}}_h\cdot\nu)(x_1,x_2)\right|}{\left[(x_1-y_1)^2+(x_2-y_2)^2\right]^{1/2}}\,d\sigma_{y_1,y_2}\,d\sigma_{x_1,x_2}.
\end{aligned}
$$

We split the double integral over $\partial(0,1)^2 \times \partial(0,1)^2$ in double integrals over $\Gamma_i \times \Gamma_j$, $i, j = 1...4$, and provide explicit computations for the cases $\Gamma_1 \times \Gamma_1$, $\Gamma_1 \times \Gamma_2$ and $\Gamma_1 \times \Gamma_3$. The other integrals can be treated similarly.

Let $\overline{p}_1$ and $\overline{p}_2$ denote the nonzero components of $\overline{\mathbf{p}}_h$. Since $\overline{\mathbf{p}}_h \cdot \nu = -\overline{p}_2$ on Γ_1, by Hölder inequality we have

$$\begin{aligned}
&\int_{\Gamma_1}\int_{\Gamma_1} \frac{\left|\left(\overline{\mathbf{p}}_h \cdot \nu\right)(y_1, y_2) - (\overline{\mathbf{p}}_h \cdot \nu)(x_1, x_2)\right|}{\left[(x_1 - y_1)^2 + (x_2 - y_2)^2\right]^{1/2}}\, d\sigma_{y_1,y_2}\, d\sigma_{x_1,x_2} \\
&\quad \leq C \left(\int_{\partial(0,1)^2 \times \partial(0,1)^2} \frac{\left|\overline{p}_2(y_1, y_2) - \overline{p}_2(x_1, x_2)\right|^2}{(x_1 - y_1)^2 + (x_2 - y_2)^2}\right)^{\frac{1}{2}}.
\end{aligned}$$

Then, since $\overline{p}_2 \in H^1\left((0,1)^2\right)$, we can apply equation (1.4) pg. 289 in Gagliardo (1957), to conclude that

$$\begin{aligned}
&\int_{\Gamma_1}\int_{\Gamma_1} \frac{\left|\left(\overline{\mathbf{p}}_h \cdot \nu\right)(y_1, y_2) - (\overline{\mathbf{p}}_h \cdot \nu)(x_1, x_2)\right|}{\left[(x_1 - y_1)^2 + (x_2 - y_2)^2\right]^{1/2}}\, d\sigma_{y_1,y_2}\, d\sigma_{x_1,x_2} \\
&\quad \leq C_1\, ||\overline{p}_2||_{H^1((0,1)^2)} \leq C_1\, ||\overline{\mathbf{p}}_h||_{H^1((0,1)^2)}.
\end{aligned}$$

On $\Gamma_1 \times \Gamma_3$, we have

$$\begin{aligned}
&\int_{\Gamma_1}\int_{\Gamma_3} \frac{\left|\left(\overline{\mathbf{p}}_h \cdot \nu\right)(y_1, y_2) - (\overline{\mathbf{p}}_h \cdot \nu)(x_1, x_2)\right|}{\left[(x_1 - y_1)^2 + (x_2 - y_2)^2\right]^{1/2}}\, d\sigma_{y_1,y_2}\, d\sigma_{x_1,x_2} \\
&= \int_0^1\int_0^1 \frac{|\overline{p}_2(y_1, 1) + \overline{p}_2(x_1, 0)|}{\sqrt{(x_1 - y_1)^2 + 1}}\, dy_1\, dx_1 \\
&\leq 2 \int_0^1\int_0^1 \frac{1}{\sqrt{(x_1 - y_1)^2 + 1}}\, dy_1\, dx_1 \\
&= 2 \int_0^1\int_{-x_1}^{1-x_1} \frac{du}{\sqrt{u^2 + 1}}\, dx_1 \leq 2 \int_0^1\int_{-1}^1 \frac{du}{\sqrt{u^2 + 1}}\, dx_1 \\
&= 4 \int_0^1\int_0^1 \frac{du}{\sqrt{u^2 + 1}}\, dx_1 = 4\, \ln(u + \sqrt{1 + u^2})\Big|_0^1 = 4 \ln(1 + \sqrt{2}).
\end{aligned}$$

Finally, on $\Gamma_1 \times \Gamma_2$ we find

$$\begin{aligned}
&\int_{\Gamma_1}\int_{\Gamma_2} \frac{\left|\left(\overline{\mathbf{p}}_h \cdot \nu\right)(y_1, y_2) - (\overline{\mathbf{p}}_h \cdot \nu)(x_1, x_2)\right|}{\left[(x_1 - y_1)^2 + (x_2 - y_2)^2\right]^{1/2}}\, d\sigma_{y_1,y_2}\, d\sigma_{x_1,x_2} \\
&= \int_0^1\int_0^1 \frac{|\overline{p}_1(1, y_2) + \overline{p}_2(x_1, 0)|}{\sqrt{(x_1 - 1)^2 + y_2^2}}\, dy_2\, dx_1 \leq 2 \int_0^1\int_0^1 \frac{1}{\sqrt{u^2 + y_2^2}}\, dy_2\, du \\
&\leq 2 \iint_{\{u^2 + y_2^2 \leq 4\}} \frac{1}{\sqrt{u^2 + y_2^2}}\, dy_2\, du = 2 \int_0^{2\pi}\int_0^2 \frac{1}{\rho}\, \rho\, d\rho\, d\theta = 8\pi.
\end{aligned}$$

And, the lemma follows. □

We are left to study the integral:

$$\int_{\partial\Omega_h}\int_{\partial\Omega_h} K_h(\mathbf{x},\mathbf{y};\mathbf{p}_h)\,\left[\left(\overline{\mathbf{p}}_h\cdot\nu\right)(\mathbf{x})\right]^2\,d\sigma_{\mathbf{y}}\,d\sigma_{\mathbf{x}}, \tag{37}$$

which we consider in the next section.

3.4 Constant Dielectric Tensor Approximation

We first analyze the term in (37) under the simplifying assumption that the tensor $\varepsilon_h^*(\mathbf{p}_h)$ in (18) is constant in $\mathbb{R}^3$ and it equals the matrix $\hat{\varepsilon}_c$ defined in (9), so that the Gauss's law that we need to study becomes

$$\nabla\cdot\left(\hat{\varepsilon}_c\,\nabla\overline{\Phi}_h\right)=\nabla\cdot(\overline{\mathbf{p}}_h\,\chi_{\Omega_h})\text{ in }\mathbb{R}^3. \tag{38}$$

By classical elliptic theory, we know the fundamental solution of (38):

$$K(\mathbf{x},\mathbf{y})=\frac{1}{4\pi}\,\frac{1}{\sqrt{\varepsilon_1\,\varepsilon_2\,\varepsilon_3}}\cdot\frac{1}{\sqrt{\frac{1}{\varepsilon_1}\,(x_1-y_1)^2+\frac{1}{\varepsilon_2}\,(x_2-y_2)^2+\frac{1}{\varepsilon_3}\,(x_3-y_3)^2}}. \tag{39}$$

Lemma 3.6 *Let $\mathbf{p}_h\in H^1(\Omega_h,S^2)$. Under our assumptions, for $i\neq j$, it holds:*

$$\lim_{h\to0}\frac{1}{h^2\,|\ln h|}\int_{\Gamma_i\times\Gamma_j}\left[\left(\overline{\mathbf{p}}_h\cdot\nu\right)(\mathbf{x})\right]^2\int_0^h\int_0^h K(\mathbf{x},\mathbf{y})=0.$$

Proof As pointed out in the proof of Lemma 3.5, for $\mathbf{x}=(x_1,x_2,x_3)\in\partial\Omega_h$ the function $(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})$ is zero when $x_3=0$ and $x_3=h$, and it depends only on x_1 and x_2 otherwise, that is on $\partial\Omega_h$ we have $(\overline{\mathbf{p}}_h\cdot\nu)(\mathbf{x})=(\overline{\mathbf{p}}_h\cdot\nu)(x_1,x_2)$.

We consider the case $i=1$, $j=2$, the other cases can be proven similarly.

For $0\le x_1\le 1$, we define

$$f_h(x_1)=\frac{\left[\left(\overline{\mathbf{p}}_h\cdot\nu\right)(x_1,0)\right]^2}{h^2\,|\ln h|}\int_{\Gamma_2}\int_0^h\int_0^h K(\mathbf{x},\mathbf{y})$$

Proceeding as in Lemma 5.1, since $\left|\overline{\mathbf{p}}_h \cdot \nu\right| \le 1$, we have a.e. in [0, 1] the bound:

$$
\begin{aligned}
&4\pi \sqrt{\varepsilon_1\,\varepsilon_2\,\varepsilon_3}\,|f_h(x_1)| \\
&\quad \le \frac{1}{|\ln h|}\int_0^1\int_0^1\int_{-v}^{1-v} \frac{\mathrm{d}u}{\sqrt{\frac{1}{\varepsilon_1}(1-x_1)^2+\frac{1}{\varepsilon_2}y_2^2+\frac{h^2}{\varepsilon_3}u^2}}\,\mathrm{d}v\,\mathrm{d}y_2 \\
&\quad \le \frac{1}{|\ln h|}\int_0^1\int_0^1\int_{-1}^{1} \frac{\mathrm{d}u\,\mathrm{d}v}{\sqrt{\frac{1}{\varepsilon_1}(1-x_1)^2+\frac{1}{\varepsilon_2}y_2^2+\frac{h^2}{\varepsilon_3}u^2}}\,\mathrm{d}y_2 \\
&\quad \le \frac{1}{|\ln h|}\int_0^1\int_0^1\int_{-1}^{1} \frac{\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}y_2}{\sqrt{\frac{1}{\varepsilon_1}(1-x_1)^2+\frac{1}{\varepsilon_2}y_2^2}} \\
&\quad = \frac{2}{|\ln h|}\int_0^1 \frac{\mathrm{d}y_2}{\sqrt{\frac{1}{\varepsilon_1}(1-x_1)^2+\frac{1}{\varepsilon_2}y_2^2}}.
\end{aligned}
$$

The changes of variable $s = \frac{x_1}{\sqrt{\varepsilon_1}}$ and $t = \frac{y_2}{\sqrt{\varepsilon_2}}$ give

$$
\begin{aligned}
&\int_0^1 \frac{1}{|\ln h|}\int_0^1 \frac{\mathrm{d}y_2}{\sqrt{\frac{1}{\varepsilon_1}(1-x_1)^2+\frac{1}{\varepsilon_2}y_2^2}}\,\mathrm{d}x_1 \\
&\quad = \frac{\sqrt{\varepsilon_1\varepsilon_2}}{|\ln h|}\int_0^{\frac{1}{\sqrt{\varepsilon_1}}}\int_0^{\frac{1}{\sqrt{\varepsilon_2}}} \frac{\mathrm{d}t\,\mathrm{d}s}{\sqrt{(\frac{1}{\sqrt{\varepsilon_1}}-s)^2+t^2}} \\
&\quad \le \frac{\sqrt{\varepsilon_1\varepsilon_2}}{|\ln h|}\int_0^{2\pi}\int_0^{M} \mathrm{d}r\,\mathrm{d}\theta \le \frac{C}{|\ln h|},
\end{aligned}
$$

where $M \ge \sqrt{\frac{1}{\varepsilon_1}+\frac{1}{\varepsilon_2}}$. And, the lemma follows. □

Lemma 3.7 *Under our assumptions, if* $\{\overline{\mathbf{p}}_h\} \subset H^1((0,1)^2)$ *converges to* $\overline{\mathbf{q}}$ *weakly in* $H^1((0,1)^2)$*, then it holds:*

$$
\begin{aligned}
&\lim_{h\to 0}\frac{3}{2}\frac{1}{h^2\,|\ln h|}\int_{\Gamma_i\times\Gamma_i}\left[\left(\overline{\mathbf{p}}_h\cdot\nu\right)(x_1,x_2)\right]^2\int_0^h\int_0^h K(\mathbf{x},\mathbf{y}) \\
&\quad = \alpha_H\int_{\Gamma_i}\left[(\overline{\mathbf{q}}\cdot\nu)(x_1,x_2)\right]^2,
\end{aligned}
$$

if $i = 1, 3$*, with* $\alpha_H = \frac{3}{4\pi\sqrt{\varepsilon_2\varepsilon_3}}$*; while*

$$
\begin{aligned}
&\lim_{h\to 0}\frac{3}{2}\frac{1}{h^2\,|\ln h|}\int_{\Gamma_i\times\Gamma_i}\left[\left(\overline{\mathbf{p}}_h\cdot\nu\right)(x_1,x_2)\right]^2\int_0^h\int_0^h K(\mathbf{x},\mathbf{y}) \\
&\quad = \alpha_V\int_{\Gamma_i}\left[(\overline{\mathbf{q}}\cdot\nu)(x_1,x_2)\right]^2,
\end{aligned}
$$

when $i = 2, 4$*, with* $\alpha_V = \frac{3}{4\pi\sqrt{\varepsilon_1\varepsilon_3}}$.

Proof We consider the case $i = 1$, the other cases can be proven similarly.

Starting as in the proof of Lemma 5.1, and making the change of variable $w = \frac{1}{\sqrt{\varepsilon_1}}(y_1 - x_1)$, we have, a.e. in $x_1 \in [0, 1]$ and for $x_2 = 0$:

$$\begin{aligned}
&\int_0^1 \int_0^h \int_0^h K(\mathbf{x}, \mathbf{y})\, \mathrm{d}y_3\, \mathrm{d}x_3\, \mathrm{d}y_1 \\
&\quad = \frac{1}{4\pi} \frac{2h^2}{\sqrt{\varepsilon_1\, \varepsilon_2\, \varepsilon_3}} \int_0^1 \int_0^1 \frac{(1-u)}{\sqrt{\frac{1}{\varepsilon_1}(x_1 - y_1)^2 + \frac{h^2}{\varepsilon_3} u^2}}\, \mathrm{d}u\, \mathrm{d}y_1 \\
&\quad = \frac{1}{4\pi} \frac{2h^2}{\sqrt{\varepsilon_1\, \varepsilon_2\, \varepsilon_3}} \sqrt{\varepsilon_1} \int_{-\frac{x_1}{\sqrt{\varepsilon_1}}}^{\frac{1-x_1}{\sqrt{\varepsilon_1}}} \int_0^1 \frac{(1-u)}{\sqrt{w^2 + \frac{h^2}{\varepsilon_3} u^2}}\, \mathrm{d}u\, \mathrm{d}w \\
&\quad = \frac{h^2}{2\pi} \frac{1}{\sqrt{\varepsilon_2\, \varepsilon_3}} \int_0^1 (1-u) \ln\left(\frac{\sqrt{\varepsilon_3}}{h\, u} \left(w + \sqrt{w^2 + \frac{h^2}{\varepsilon_3} u^2} \right) \right) \Bigg|_{w=-\frac{x_1}{\sqrt{\varepsilon_1}}}^{w=\frac{1-x_1}{\sqrt{\varepsilon_1}}} \mathrm{d}u \\
&\quad = \frac{h^2}{2\pi} \frac{1}{\sqrt{\varepsilon_2\, \varepsilon_3}} \int_0^1 H_h(x_1, u)\, \mathrm{d}u,
\end{aligned}$$

here we use

$$\begin{aligned}
H_h(x_1, u) &= (1-u) \ln\left(w + \sqrt{w^2 + \frac{h^2}{\varepsilon_3} u^2} \right) \Bigg|_{w=-\frac{x_1}{\sqrt{\varepsilon_1}}}^{w=\frac{1-x_1}{\sqrt{\varepsilon_1}}} \\
&= \left| \ln\left(\frac{h}{\sqrt{\varepsilon_3}} \right) \right| (H_h^1 - H_h^2),
\end{aligned}$$

where H_h^1 and H_h^2 are defined and studied in Lemma 5.2 and 5.3, respectively.

Using the notations in Lemmas 5.2 and 5.3, we have

$$\begin{aligned}
&\frac{3}{2} \frac{1}{h^2\, |\ln h|} \int_{\Gamma_1 \times \Gamma_1} \left[\left(\overline{\mathbf{p}}_h \cdot \nu \right)(x_1, 0) \right]^2 \int_0^h \int_0^h K(\mathbf{x}, \mathbf{y}) \\
&\quad = \frac{3}{2} \frac{1}{h^2\, |\ln h|} \int_0^1 \left[\left(\overline{\mathbf{p}}_h \cdot \nu \right)(x_1, 0) \right]^2 \int_0^1 \int_0^h \int_0^h K(\mathbf{x}, \mathbf{y})\, \mathrm{d}y_3\, \mathrm{d}x_3\, \mathrm{d}y_1\, \mathrm{d}x_1 \\
&\quad = \alpha_H \frac{1}{|\ln h|} \int_0^1 \left[\left(\overline{\mathbf{p}}_h \cdot \nu \right)(x_1, 0) \right]^2 \int_0^1 H_h(x_1, u)\, \mathrm{d}u\, \mathrm{d}x_1 \\
&\quad = \alpha_H \frac{\left| \ln\left(\frac{h}{\sqrt{\varepsilon_3}} \right) \right|}{|\ln h|} \int_0^1 \left[\left(\overline{\mathbf{p}}_h \cdot \nu \right)(x_1, 0) \right]^2 \int_0^1 \left[H_h^1(x_1, u) - H_h^2(x_1, u) \right] \mathrm{d}u\, \mathrm{d}x_1.
\end{aligned}$$

We note that $\left[\left(\overline{\mathbf{p}}_h \cdot \nu \right)(x_1, 0) \right]^2 \leq 1$ and that $\{\overline{\mathbf{p}}_h\}$ converges to $\overline{\mathbf{q}}$ in $L^2(\Gamma_1)$, by uniqueness of limit and compactness of the trace operator on Lipschitz domains, since weakly convergent sequences are bounded. Also, by Lemmas 5.2 and 5.3 in the Appendix, the Lebesgue Dominated Convergence Theorem implies that $\int_0^1 H_h^1(\cdot, u)\,\mathrm{d}u \to 0$ and $\int_0^1 H_h^2(\cdot, u)\,\mathrm{d}u \to \int_0^1 -2(1-u)\,\mathrm{d}u = -1$, as $h \to 0$. Thus, Lemma 5.4 in the Appendix gives

$$\frac{\alpha_H}{|\ln h|}\left[(\overline{\mathbf{p}}_h \cdot \nu)(x_1, 0)\right]^2 H_h(x_1, u) \longrightarrow \alpha_H \left[(\overline{\mathbf{q}} \cdot \nu)(x_1, 0)\right]^2$$

in $L^1((0,1)^2)$ as $h \to 0$, and the lemma follows. □

3.5 Materials with Constant Relative Dielectric Tensor

As a consequence of inequality (24), the analogous of Lemma 3.6 holds for a general $\varepsilon_h^*(\mathbf{p}_h)$ - see Lemma 3.8 below. A weaker version of Lemma 3.7 can be derived for the case of a material with relative dielectric tensor independent of $\mathbf{p}_h$, that is when $\varepsilon_h^*(\mathbf{p}_h) = \hat{\varepsilon}_{pc}$ for

$$\hat{\varepsilon}_{pc}(\mathbf{x}) = \begin{cases} \hat{\varepsilon}_c(\mathbf{x}) & \text{in } \Omega_h \\ I & \text{outside } \Omega_h. \end{cases} \tag{40}$$

Note that for this choice (25) becomes

$$\nabla \cdot \left(\hat{\varepsilon}_{pc} \nabla \overline{\Phi}_h\right) = \nabla \cdot (\overline{\mathbf{p}}_h \chi_{\Omega_h}) \text{ in } \mathbb{R}^3. \tag{41}$$

In the following, we denote by $K_h(\mathbf{x}, \mathbf{y})$ the fundamental solution of (41).

Lemma 3.8 *Let $\mathbf{p}_h \in H^1(\Omega_h, S^2)$. Under our assumptions, for $i \neq j$, it holds:*

$$\lim_{h \to 0} \frac{1}{h^2 |\ln h|} \int_{\Gamma_i \times \Gamma_j} \left[\left(\overline{\mathbf{p}}_h \cdot \nu\right)(\mathbf{x})\right]^2 \int_0^h \int_0^h K_h(\mathbf{x}, \mathbf{y}; \mathbf{p}_h) = 0.$$

Proof By (24), we have that

$$\left|\lim_{h \to 0} \frac{1}{h^2 |\ln h|} \int_{\Gamma_i \times \Gamma_j} \left[\left(\overline{\mathbf{p}}_h \cdot \nu\right)(\mathbf{x})\right]^2 \int_0^h \int_0^h K_h(\mathbf{x}, \mathbf{y}; \mathbf{p}_h)\right|$$
$$\leq C \lim_{h \to 0} \frac{1}{h^2 |\ln h|} \int_{\Gamma_i \times \Gamma_j} \left[\left(\overline{\mathbf{p}}_h \cdot \nu\right)(\mathbf{x})\right]^2 \int_0^h \int_0^h \frac{1}{|\mathbf{x} - \mathbf{y}|},$$

and the same proof as the one of Lemma 3.6 can follow to obtain that the limit on the right-hand side tends to zero. □

To study the nonzero contribution of the boundary term, we apply the classical Dunford-Pettis theorem (see for example Theorem 1.38 pg 18 in Ambrosio et al. (2000)) and Lemma 5.4 in the Appendix.

Lemma 3.9 *Under our assumptions and when $\varepsilon_h^*(\mathbf{p}_h) \equiv \hat{\varepsilon}_{pc}$, there exist $\{h_j\} \subset \{h\}$ and $\alpha_i \in L^1(\Gamma_i)$ $i = 1..4$, such that if $\{\mathbf{p}_h\} \subset H^1(\Omega_h, S^2)$ is such that $\{\overline{\mathbf{p}}_h\} \subset H^1((0,1)^2)$ converges to $\overline{\mathbf{q}}$ weakly in $H^1((0,1)^2)$, then it holds:*

$$\lim_{h_j \to 0} \frac{1}{h_j^2\,|\ln h_j|} \int_{\Gamma_i \times \Gamma_i} \left[\left(\overline{\mathbf{p}}_{h_j} \cdot \nu\right)(x_1, x_2)\right]^2 \int_0^{h_j} \int_0^{h_j} K_{h_j}(\mathbf{x}, \mathbf{y}) = \int_{\Gamma_i} \alpha_i(x_1, x_2) \left[(\overline{\mathbf{q}} \cdot \nu)(x_1, x_2)\right]^2. \tag{42}$$

Proof Let $i = 1$. We set $f_h = (\overline{\mathbf{p}}_h \cdot \nu)^2$ and

$$g_h = \frac{1}{h^2 |\ln h|} \int_0^1 \int_0^h \int_0^h K_h(\mathbf{x}, \mathbf{y})\, dy_3\, dx_3\, dy_1.$$

By compactness of the trace operator, we have that $f_h \to (\overline{\mathbf{q}} \cdot \nu)^2$ in $L^1(\Gamma_1)$ and $|f_h| \leq 1$. Proceeding as in Lemma 3.7, the upper bound in (24), using Lemmas 5.2 and 5.3, gives that $\{g_h\} \subset L^1(\Gamma_1)$ and that g_h is dominated by an L^1 function. From this, the Dunford-Pettis theorem provides the existence of a subsequence that converges weakly in L^1, that is there is a subsequence $\{g_{h_j}\}$ and an $\alpha_1 \in L^1(\Gamma_1)$ such that $g_{h_j} \rightharpoonup \alpha_1$ in $L^1(\Gamma_1)$. Note that α_1 and the subsequence $\{h_j\}$ do not depend on the sequence $\mathbf{p}_h$. And, (42) follows for $i = 1$ from Lemma 5.4 in the Appendix. Repeating the argument for $i = 2$, starting from the subsequence h_j and so on, since the index i ranges within a finite set, we obtain the lemma, with the α_i being independent of the choice of the sequence $\mathbf{p}_h$. ◻

4 Dimensional Reduction

We use the estimates obtained in Sect. 3 to derive via Γ-convergence two-dimensional reduced energy functionals, starting from a rescaled version of (17). Namely, for $h > 0$, we consider $\{\mathbf{p}_h\} \in H^1(\Omega_h, S^2)$, $\mathbf{p}_h = (p_1^h, p_2^h, 0)$, and the energy:

$$\begin{aligned} E_h(\mathbf{p}_h) &= \frac{\mathcal{E}_h(\mathbf{p}_h)}{h^2 |\ln h|} \\ &\equiv \frac{\epsilon_0}{2 P_0^2\, L^2}\, \frac{K_G}{h\,|\ln h|} \int_{\Omega_1} \Big[|\nabla' \widetilde{\mathbf{p}}_h|^2 + \frac{-2\,k_T^*}{h}\, \widetilde{\mathbf{p}}_h^{\perp} \cdot \partial_3 \widetilde{\mathbf{p}}_h + \frac{K_T^* + 1}{h^2}\, |\partial_3 \widetilde{\mathbf{p}}_h|^2 \\ &\quad + K_S^* \left(\mathrm{div}' \widetilde{\mathbf{p}}_h\right)^2 + K_B^* (\mathrm{curl}' \widetilde{\mathbf{p}}_h)^2 + 2\, c_p^*\ \mathrm{div}' \widetilde{\mathbf{p}}_h - 2\, \sigma_s\, \sigma\, \widetilde{\mathbf{p}}_h \cdot \mathbf{e} \Big] \\ &\quad + \frac{1}{h^2 |\ln h|} \int_{\mathbb{R}^3} \frac{3}{2} \varepsilon_h^*(\mathbf{p}_h)\, \nabla \Phi_h \cdot \nabla \Phi_h, \end{aligned} \tag{43}$$

with

$$\nabla \cdot \left(\varepsilon_h^*(\mathbf{p}_h)\, \nabla \Phi_h\right) = \nabla \cdot (\mathbf{p}_h\, \chi_{\Omega_h}) \quad \text{in } \mathbb{R}^3, \tag{44}$$

and define

$$E(\mathbf{r})=\begin{cases}\beta\int_{(0,1)^2}e(\mathbf{r})+\int_{\partial(0,1)^2}w(\mathbf{x};\mathbf{r};\nu) & \text{if } \mathbf{r}(\mathbf{x})=\mathbf{r}(x_1,x_2) \text{ and } r_3=0,\\ \infty & \text{otherwise,}\end{cases} \tag{45}$$

where $\beta>0$,

$$e(\mathbf{r})=|\nabla\mathbf{r}|^2+K_S^*(\operatorname{div}\mathbf{r})^2+K_B^*(\operatorname{curl}\mathbf{r})^2-2\sigma_s\,\sigma\,\mathbf{r}\cdot\mathbf{e}, \tag{46}$$

and

$$w(\mathbf{x};\mathbf{r};\nu)=\alpha(\mathbf{x})\,(\mathbf{r}\cdot\nu)^2+2c_p^*\,\mathbf{r}\cdot\nu, \tag{47}$$

for some $\alpha\in L^1(\Gamma_i)$, $i=1,\ldots,4$.

Given a generalized sequence $\{\eta\}$ of real positive numbers or of integers, we say that the family of functionals $\{E_\eta\}$ Γ-converges to E weakly in $H^1(\Omega_1,S^2)$ if

1. (Liminf inequality) Given $\{\mathbf{p}_\eta\}\subset H^1(\Omega_\eta,S^2)$, such that $\widetilde{\mathbf{p}}_\eta$ converges weakly to $\mathbf{q}$ in $H^1(\Omega_1,S^2)$ then $\liminf_{\eta\to 0}E_\eta(\mathbf{p}_\eta)\geq E(\mathbf{q})$.
2. (Limsup inequality) For any $\mathbf{q}\in H^1(\Omega_1,S^2)$, there exists $\{\mathbf{p}_\eta\}\subset H^1(\Omega_\eta,S^2)$ such that $\widetilde{\mathbf{p}}_\eta$ converges weakly to $\mathbf{q}$ in $H^1(\Omega_1,S^2)$ and $E(\mathbf{q})=\lim_{\eta\to 0}E(\mathbf{p}_\eta)$.

We then have the following main result:

Theorem 4.1 *Let $h>0$ and $\{\mathbf{p}_h\}\subset H^1(\Omega_h,S^2)$ with $\mathbf{p}_h=(p_1^h,p_2^h,0)$. Assume that as $h\to 0$ it holds that $\frac{\epsilon_0}{2P_0^2L^2}\frac{K_G}{h\,|\ln h|}\to\beta>0$, and that there exist $h_0>0$ and $C>0$ such that $E_h(\mathbf{p}_h)\leq C$ for all $h<h_0$. Then, there exists a subsequence (not relabeled) and $\mathbf{q}\in H^1(\Omega_1,S^2)$, with $\mathbf{q}(\mathbf{x})=\mathbf{q}(x_1,x_2)$ and $q_3=0$, such that*

$$\widetilde{\mathbf{p}}_h\rightharpoonup\mathbf{q}\quad\textit{weakly in } H^1(\Omega_1,S^2). \tag{48}$$

Additionally, we distinguish the two following cases:

***Case I**: If the dielectric tensor $\varepsilon_h^*(\mathbf{x})$ is independent of $\mathbf{p}_h$, i.e., $\varepsilon_h^*(\mathbf{p}_h)=\hat{\varepsilon}_{pc}$ (40), then there exists a sequence $\{h_j\}$ such that $\{E_{h_j}\}$ Γ-converges to E weakly in $H^1(\Omega_1,S^2)$ with $\alpha(\mathbf{x})=\alpha_i(\mathbf{x})\in L^1(\Gamma_i)$ for $\mathbf{x}\in\Gamma_i$ and $i=1,\ldots,4$, where the functions α_i and the sequence $\{h_j\}$ are as in Lemma 3.9.*

***Case II**: If the dielectric tensor is a constant diagonal matrix, i.e., $\varepsilon_h^*(\mathbf{p}_h)=\hat{\varepsilon}_c$ (9), then $\{E_h\}$ Γ-converges to E weakly in $H^1(\Omega_1,S^2)$, where $\alpha=\frac{3}{4\pi\sqrt{\varepsilon_2\varepsilon_3}}$ on Γ_1 and Γ_3 and $\alpha=\frac{3}{4\pi\sqrt{\varepsilon_1\varepsilon_3}}$ on Γ_2 and Γ_4.*

Proof Case II: Assume $\varepsilon_h^*(\mathbf{p}_h)=\hat{\varepsilon}_c$, from $E_h(\mathbf{p}_h)\leq C$, $\widetilde{\mathbf{p}}_h$ converges up to a subsequence weakly in $H^1(\Omega_1,S^2)$ to some $\mathbf{q}\in H^1(\Omega_1,S^2)$. By rewriting, up to additive constants, the energy in the following form:

$$
\begin{aligned}
E_h(\mathbf{p}_h) = & \frac{\epsilon_0}{2P_0^2\, L^2} \frac{K_G}{h\,|\ln h|} \int_{\Omega_1} \left[\frac{K_T^*+1}{h^2} \left| \partial_3 \widetilde{\mathbf{p}}_h - \frac{k_T^*\, h}{K_T^*+1} \widetilde{\mathbf{p}}_h^{\perp} \right|^2 \right. \\
& \left. + K_S^* \left(\mathrm{div}' \widetilde{\mathbf{p}}_h + \frac{c_p}{K_S^*} \right)^2 + K_B^* (\mathrm{curl}' \widetilde{\mathbf{p}}_h)^2 + |\nabla' \widetilde{\mathbf{p}}_h|^2 - 2\,\sigma_s\,\sigma\, \widetilde{\mathbf{p}}_h \cdot \mathbf{e} \right] \\
& + \frac{1}{h^2|\ln h|} \int_{\mathbb{R}^3} \frac{3}{2} \varepsilon_h^*(\mathbf{p}_h)\, \nabla \Phi_h \cdot \nabla \Phi_h,
\end{aligned}
$$

we see that $\liminf E_h(\mathbf{p}_h) \geq E(\mathbf{q})$ for any $\mathbf{p}_h \rightharpoonup \mathbf{q}$ in $H^1(\Omega_1, S^2)$, from (31) and Lemmas 3.3–3.7. On the other hand, for any $\mathbf{q} \in H^1(\Omega_1, S^2)$ we can construct a sequence by taking $\mathbf{p}_h = \mathbf{q}$ to show $\limsup E_h(\mathbf{p}_h) = E(\mathbf{q})$. Case I follows by a similar proof applied now to the subsequence $\{E_{h_j}\}$. □

5 Numerical Approximation

5.1 Ferroelectric Polar Smectic A Liquid Crystals SmAP$_F$

For our numerical simulation of the SmAP$_F$ phase, we use the one-constant approximation, that is we take $K_S = K_B = K_T = K_G$, and consider a relaxation of the energy, which depends on a small parameter ϵ. The first is an assumption often found in the physics literature, the second is a numerical device frequently found in numerical works, which is used to relax the unit-length constraint. Finally, since the explicit form of the function $\alpha(\mathbf{x})$ in Theorem 4.1 is not known, we take it to be piecewise constant with the same values on the horizontal and vertical sides - this form is suggested by the result in Lemma 3.7 of the simplified case studied in section 3.4. In non-dimensional units, the energy numerically studied looks like

$$
\begin{aligned}
E_\epsilon(\mathbf{p}) = & \int_\Omega \left(|\nabla \mathbf{p}|^2 - 2\sigma_s\,\sigma\, p_2 + \frac{(1-|\mathbf{p}|^2)^2}{2\epsilon^2} \right) d\mathbf{x} \\
& + \omega_V \int_{\Gamma_V} (\mathbf{p}\cdot\nu + a)^2\, d\sigma + \omega_H \int_{\Gamma_H} (\mathbf{p}\cdot\nu + b)^2\, d\sigma,
\end{aligned}
\tag{49}
$$

where $\mathbf{p} = (p_1, p_2)$,

$$
\Omega = (0,1)^2;\;\; \Gamma_H = (0,1)\times\{0,1\};\;\; \Gamma_V = \{0,1\}\times(0,1),
$$

and $\sigma = \dfrac{L^2\, P_0\,|E_{ex}|}{K_G}$ is proportional to the intensity of the applied electric field. Note that from the derivation of our model we have the condition $\omega_V\, a = \omega_H\, b$.

We take $\sigma_s = 1$, and consider the gradient flow for (49), $\mathbf{p}_t = -\dfrac{\delta E_\epsilon}{\delta \mathbf{p}}$. The resulting system of equations is

$$
\begin{cases}
\dfrac{\partial \mathbf{p}}{\partial t} = \Delta \mathbf{p} + \begin{pmatrix} 0 \\ \sigma \end{pmatrix} \mathbf{p} + \dfrac{(1 - |\mathbf{p}|^2)}{\epsilon^2} \mathbf{p} & \text{in } \Omega \\
\dfrac{\partial \mathbf{p}}{\partial \nu} = -\omega_V \left(\mathbf{p} \cdot \nu + a \right) \nu & \text{on } \Gamma_V \\
\\
\dfrac{\partial \mathbf{p}}{\partial \nu} = -\omega_H \left(\mathbf{p} \cdot \nu + b \right) \nu & \text{on } \Gamma_H .
\end{cases} \tag{50}
$$

We discretize the system in time using a semi-implicit method, with a second-order backward differentiation formula for the Laplacian part, and an explicit second-order formula for the nonlinear terms. We use the standard second-order discretization for the Laplacian in space, and solve the resulting linear system of equations using the discrete Fourier Transform.

We then run the simulation with the following choice of parameters:

$$
\epsilon = 0.02, \ \omega_V = \frac{1}{\epsilon^{3/2}}, \ \omega_H = \frac{1}{\epsilon}, \ a = \sqrt{\epsilon}, \ b = 1.
$$

In the $\mathrm{SmAP_F}$ phase, the polar ordering is not uniform in the ground state, as polarization splay occurs due to the surface energy. The one-dimensional study presented in Guo et al. (2011) shows the molecules near the surface pointing either toward or out of the top and bottom glass plates and an horizontal polarization in the middle of the sample to accommodate the boundary conditions at the top and bottom. The same behavior is obtained in the two-dimensional case, as shown in Fig. 1a. In addition, in this two-dimensional confined geometry, with our choice of parameters, we see a pair of boundary vortices appearing, with the molecules preferring to be almost parallel to the lateral segment of the domain boundary. The application of an upward electric field results in the vortices moving upward so that more polarization fields in the domain point upward (Fig. 1b, c). When a sufficiently high electric field is applied, the bent-core molecules reorient following the direction of the electric field in most part of the domain (Fig. 1d).

Note that to compare our results with the numerical pictures for the polar director profiles presented in the one-dimensional approximation of Gornik et al. (2014), in Fig. 1, we take the positive y-axis to be in the horizontal direction pointing to the right, and the positive x-axis in the vertical one pointing upwards, and plot the polar director. The one-dimensional approximation is consistent with the behavior of the polar director at the center of the sample.

5.2 Bistability Behavior of $\mathrm{SmAP_{Fmod}}$

In García-Cervera et al. (2020), we studied the ferroelectric bistability of the polarization-modulated orthogonal smectic liquid crystals described first in Zhu et al. (2012). To model the $\mathrm{SmAP_{Fmod}}$ phase, we considered the following relaxed energy functional:

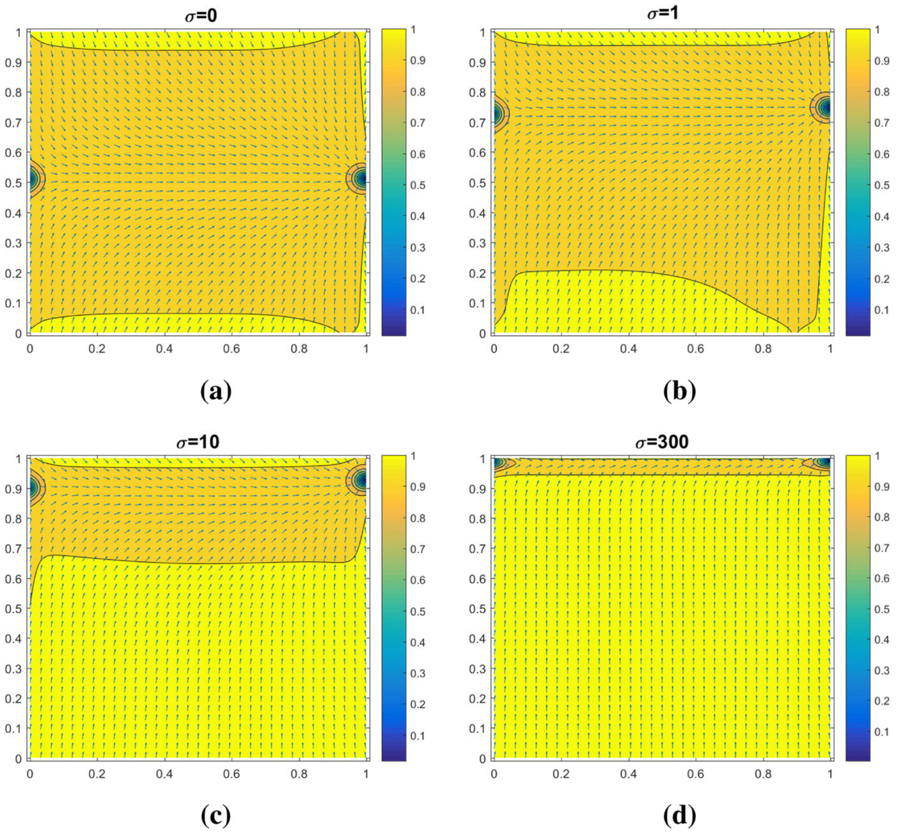

Fig. 1 Numerical solution of the gradient flow (50) for $\sigma = 0, 1, 10, 300$ with $\varepsilon = 0.02$

$$\mathcal{F}_\varepsilon(\mathbf{p}) = \frac{1}{2}\int_\Omega \left(|\nabla \mathbf{p}|^2 + \frac{1}{2\varepsilon^2}(1-|\mathbf{p}|^2)^2 + \sigma|\mathbf{e}-\mathbf{p}|^2 \right) dxdy + \frac{1}{2\varepsilon}\int_{\Gamma_H} (\mathbf{p}\cdot\nu)^2\, dx, \tag{51}$$

where $\mathbf{e} = \sigma_s\, \mathbf{e}_2$, $\Omega = (0,1)^2$, and $\Gamma_H = (0,1)\times\{0,1\}$ and imposed a Dirichlet boundary condition for $\mathbf{p}$ on the vertical sides:

$$\mathbf{p} = \nu \qquad \text{for } \mathbf{x} \in \Gamma_V = \{0,1\}\times(0,1), \tag{52}$$

where ν is the outward normal vector, and defined

$$H^1_D = \left\{ \mathbf{p} \in H^1(\Omega;\mathbb{R}^2) : \mathbf{p}|_{\Gamma_V} = \nu \right\}. \tag{53}$$

We were able to prove that as $\varepsilon \to 0$ the global energy minimizers in H^1_D of E_ε converge up to subsequences to an S^1 valued function, which has always boundary vortices. We also numerically studied the dynamics of the model bistability, by reversing the direction of the applied electric field. Unlike the model proposed in Zhu et al. (2012), where the authors expected the switching to happen with the nucleation of one internal vortex, our simulations shows the formation of two distinct internal vortices, which move towards the center of the sample, where they annihilate each other.

In here, we consider the non-equal elastic constant case:

$$F_\epsilon(\mathbf{p}) = \int_\Omega \left(k_1^*(\nabla \cdot \mathbf{p})^2 + k_2^*|\nabla \times \mathbf{p}|^2 + a|\nabla \mathbf{p}|^2 + \frac{1}{2\varepsilon^2}(1 - |\mathbf{p}|^2)^2 \right.$$
$$\left. + \sigma|\mathbf{p} - \mathbf{e}|^2 \right) d\mathbf{x} + \frac{1}{\varepsilon}\int_{\Gamma_H} (\mathbf{p} \cdot \nu)^2, \tag{54}$$

and the same Dirichlet boundary condition for **p** on the vertical sides.

This energy with zero electric field, on a smooth domain, and with nonzero degree Dirichlet data on all of the boundary was studied analytically in Colbert-Kelly and Phillips (2013), and numerically in Colbert-Kelly et al. (2017) to investigate the vortex configurations. We follow the numerical scheme provided in Colbert-Kelly et al. (2017). The gradient flow of the energy can be written for each case, $k_1^* \geq k_2^*$ and $k_2^* \geq k_1^*$, separately:

$$\frac{\partial p}{\partial t} = \mathcal{L}(\mathbf{p}) + \frac{1}{\varepsilon^2}(1 - |\mathbf{p}|^2)\mathbf{p} + \sigma(\mathbf{e}_2 - \mathbf{p}), \tag{55}$$

where

$$\mathcal{L}(\mathbf{p}) = \begin{cases} (a + k_2^*)\Delta\mathbf{p} - (k_2^* - k_1^*)\nabla(\nabla \cdot \mathbf{p}) & \text{if } k_2^* > k_1^* \\ (a + k_1^*)\Delta\mathbf{p} - (k_2^* - k_1^*)\nabla \times (\nabla \times \mathbf{p}) & \text{if } k_1^* > k_2^*, \end{cases}$$

with boundary conditions

$$a\frac{\partial \mathbf{p}}{\partial \nu} + k_1^*(\nabla \cdot \mathbf{p})\nu + k_2^*(\nabla \times \mathbf{p}) \times \nu + \frac{1}{\varepsilon}(\mathbf{p} \cdot \nu)\nu = 0 \quad \text{on } \Gamma_H,$$
$$\mathbf{p} = \nu \quad \text{on } \Gamma_V.$$

During the switching process, Fig. 2 shows that only one internal vortex appears to reverse the polarization. This is different from what we observed in the equal constant case, $k_1^* = k_2^*$, where two interior vortices nucleate from each boundary vortex and they meet in the middle of the sample and then annihilate each other. We take $k_1^* = 1$, $k_2^* = 0.7$, and $a = 0.3$, since according to the physics literature in BLCs the splay elastic constant is larger than the bend elastic constant (Majumdar et al. 2011; Gornik et al. 2014). Initially $-1/2$ and $1/2$ vortices appear at the top and bottom surfaces, respectively (see Fig. 2a). Then, Fig. 2b and c shows that the $-1/2$ vortex at (0.5, 1) splits into a $1/2$ vortex at the boundary and a -1 interior vortex. This -1 interior vortex starts moving downward (see Fig. 2c–e) and is eventually expelled, by the combination with the $+1/2$ vortex at the bottom surface (Fig. 2f). This completes the switching process and we now see one $-1/2$ boundary vortex on the bottom plate and the polarization pointing downward in most part of the domain.

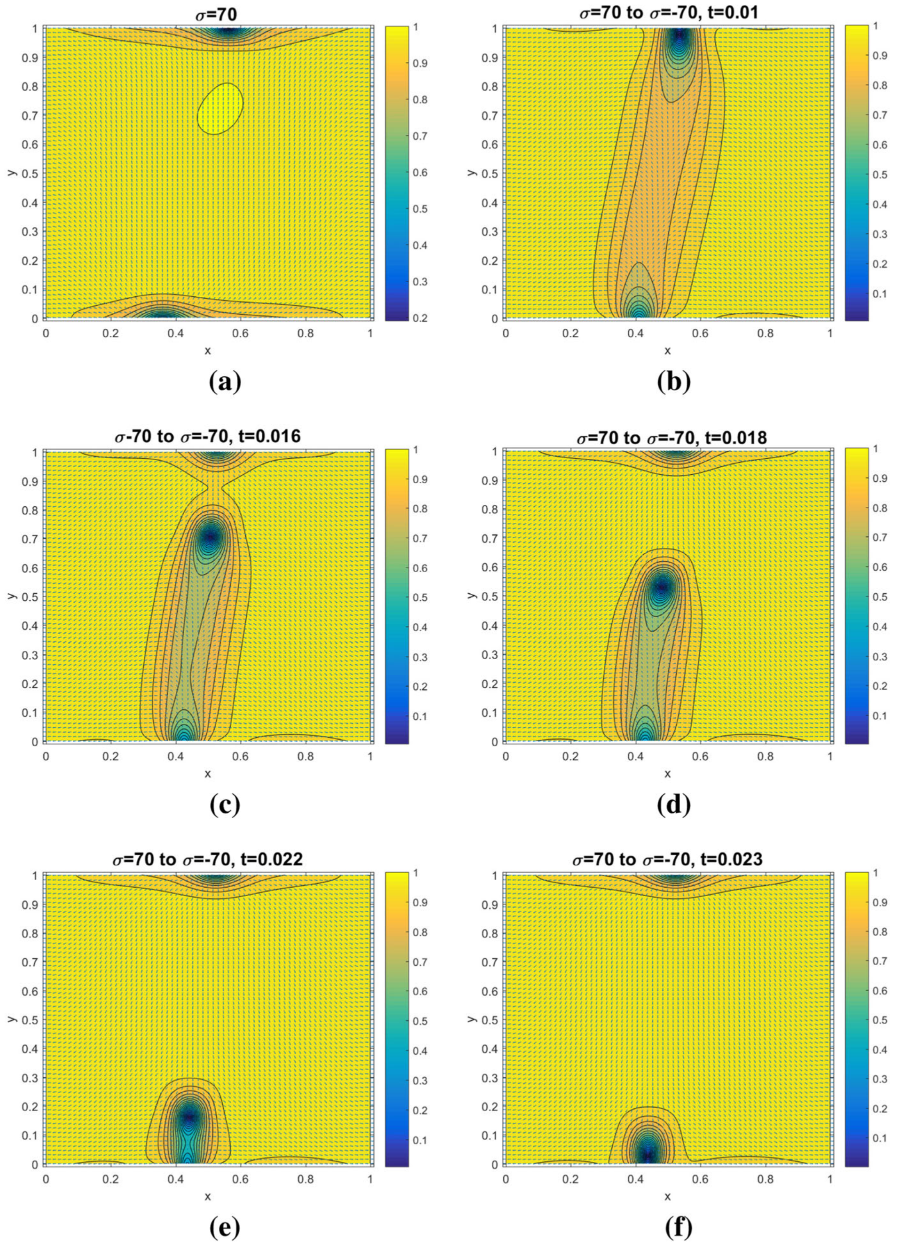

Fig. 2 Numerical solution of the gradient flow (55) for switching dynamics from $\sigma = 70$ to $\sigma = -70$, with $\varepsilon = 0.03$. The polarization fields are depicted at selected times $t = 0, t = 0.01, t = 0.016, t = 0.018, t = 0.022, t = 0.023$

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Data Availability Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

Declarations

Conflict of interest The authors declare that there is no conflict of interest.

Appendix

For the convenience of the reader, in this section we provide some computations concerning the limits used in Lemmas 3.6 and 3.7.

Lemma 5.1 *Let* $A > 0$*, then if* $h, \varepsilon_3 > 0$*, we have*

$$\int_0^h \int_0^h \frac{dy_3\, dx_3}{\sqrt{A + \frac{1}{\varepsilon_3}(x_3 - y_3)^2}} = I_h(A) - J_h(A),$$

where

$$I_h(A) = 2h\sqrt{\varepsilon_3}\left[\ln\left(\frac{h}{\sqrt{\varepsilon_3}} + \sqrt{A + \frac{h^2}{\varepsilon_3}}\right) - \ln\sqrt{A}\right]$$

and

$$J_h(A) = 2\,\varepsilon_3\left(\sqrt{A + \frac{h^2}{\varepsilon_3}} - \sqrt{A}\right).$$

Proof We follow Carbou (2001), and use the change of variables $h\,v = x_3$, and $h\,u = y_3 - h\,v$ to gather

$$\begin{aligned}\int_0^h \int_0^h \frac{\mathrm{d}y_3\, \mathrm{d}x_3}{\sqrt{A + \frac{1}{\varepsilon_3}(x_3 - y_3)^2}} &= h\int_0^1 \int_0^h \frac{\mathrm{d}y_3\, \mathrm{d}v}{\sqrt{A + \frac{1}{\varepsilon_3}(h\,v - y_3)^2}} \\ &= h^2 \int_0^1 \int_{-v}^{1-v} \frac{\mathrm{d}u\, \mathrm{d}v}{\sqrt{A + \frac{h^2}{\varepsilon_3}u^2}}.\end{aligned}$$

Changing the order of integration, and computing the integral in v, then yields

$$\int_0^h \int_0^h \frac{\mathrm{d}y_3\, \mathrm{d}x_3}{\sqrt{A + \frac{1}{\varepsilon_3}(x_3 - y_3)^2}} = 2\,h^2 \int_0^1 \frac{(1-u)}{\sqrt{A + \frac{h^2}{\varepsilon_3}u^2}}\mathrm{d}u.$$

Computing the integral in u gives the desired equality. $\square$

Lemma 5.2 *Let $(x_1, u) \in [0, 1]^2$, then a.e. we have*

$$\lim_{h \to 0} H_h^1(x_1, u) = 0,$$

where

$$H_h^1(x_1, u) := \frac{1-u}{|\ln(\frac{h}{\sqrt{\varepsilon_3}})|} \ln\left[\frac{1-x_1}{\sqrt{\varepsilon_1}} + \sqrt{\frac{(1-x_1)^2}{\varepsilon_1} + \frac{h^2}{\varepsilon_3}u^2}\right].$$

Additionally, there exist $h_1(\varepsilon_1, \varepsilon_3) > 0$, and $H^1(x_1, u) \in L^1((0, 1)^2)$, such that, for $0 < h < h_1$, a.e. it holds

$$|H_h^1(x_1, u)| \leq H_1(x_1, u).$$

Proof If $(x_1, u) \neq (1, 0)$, as $\frac{h}{\sqrt{\varepsilon_3}} \to 0$, the numerator of $H_h^1 \to (1-u) \ln\left[\frac{2(1-x_1)}{\sqrt{\varepsilon_1}}\right]$, while the denominator tends to infinity, hence $H_h^1(x_1, u) \to 0$ a.e. in $[0, 1]^2$.

Let $h_1 > 0$ be such that, $\frac{\varepsilon_1}{\varepsilon_3} h_1^2 < 1$, and $\frac{h}{\sqrt{\varepsilon_3}} < 1$, and set $\gamma_1 = \frac{1}{2}(\frac{\varepsilon_1}{\varepsilon_3} h_1^2 + 1)$. Then, if $0 < h < h_1$, $0 \leq u \leq 1$, and $0 \leq x_1 \leq \gamma_1$, we have

$$\begin{aligned}
&\left|\ln\left[\frac{1-x_1}{\sqrt{\varepsilon_1}} + \sqrt{\frac{(1-x_1)^2}{\varepsilon_1} + \frac{h^2}{\varepsilon_3}u^2}\right]\right| \\
&\quad = \left|\ln \frac{1}{\sqrt{\varepsilon_1}} + \ln\left[1 - x_1 + \sqrt{(1-x_1)^2 + \frac{\varepsilon_1}{\varepsilon_3} h^2 u^2}\right]\right| \leq \frac{1}{2} |\ln \varepsilon_1| + C_0,
\end{aligned}$$

where

$$C_0 = \max\left\{\left|\ln\left[1 - x_1 + \sqrt{(1-x_1)^2 + \frac{\varepsilon_1}{\varepsilon_3} h^2 u^2}\right]\right|\right\},$$

max taken over $0 < h < h_1, 0 \leq u \leq 1,$ and $0 \leq x_1 \leq \gamma_1$.

On the other hand, if $\frac{1}{2}(\frac{\varepsilon_1}{\varepsilon_3} h_1^2 + 1) < x_1 \leq 1$, whenever $(x_1, u) \neq (1, 0)$, we have

$$0 \leq 1 - x_1 + \sqrt{(1-x_1)^2 + \frac{\varepsilon_1}{\varepsilon_3} h^2 u^2} \leq 1,$$

and, $0 \leq 2(1 - x_1) \leq 1$. Therefore,

$$\left|\ln\left[1 - x_1 + \sqrt{(1-x_1)^2 + \frac{\varepsilon_1}{\varepsilon_3} h^2 u^2}\right]\right| \leq |\ln 2(1 - x_1)|.$$

And, the lemma follows with

$$H_1(x_1,u) = \begin{cases} C_1 \frac{1-u}{|\ln(\frac{h_1}{\sqrt{\varepsilon_3}})|} & \text{if } 0 \le x_1 \le \gamma_1; \\ \frac{1-u}{|\ln(\frac{h_1}{\sqrt{\varepsilon_3}})|}(C_2 + |\ln(1-x_1)|) & \text{if } \gamma_1 < x_1 < 1. \end{cases}$$

where $C_1 = \frac{1}{2}|\ln \varepsilon_1| + C_0$, and $C_2 = \frac{1}{2}|\ln \varepsilon_1| + \ln 2$. □

Lemma 5.3 *Let* $(x_1, u) \in [0, 1]^2$*, then a.e. we have*

$$\lim_{h \to 0} H_h^2(x_1, u) = -2(1-u),$$

where

$$H_h^2(x_1,u) := \frac{1-u}{|\ln(\frac{h}{\sqrt{\varepsilon_3}})|} \ln\left[\frac{-x_1}{\sqrt{\varepsilon_1}} + \sqrt{\frac{x_1^2}{\varepsilon_1} + \frac{h^2}{\varepsilon_3}u^2}\right].$$

Additionally, we can find $h_2(\varepsilon_1, \varepsilon_3) > 0$*, and* $H_2(x_1, u) \in L^1((0, 1)^2)$*, such that, for* $0 < h < h_2$*, a.e. it holds*

$$|H_h^2(x_1,u)| \le H_2(x_1,u).$$

Proof If $u \neq 0$, we can rewrite the logarithmic part as

$$\begin{aligned} \ln\left[\frac{-x_1}{\sqrt{\varepsilon_1}} + \sqrt{\frac{x_1^2}{\varepsilon_1} + \frac{h^2}{\varepsilon_3}u^2}\right] &= \ln\left[\frac{\frac{h^2}{\varepsilon_3}u^2}{\frac{x_1}{\sqrt{\varepsilon_1}} + \sqrt{\frac{x_1^2}{\varepsilon_1} + \frac{h^2}{\varepsilon_3}u^2}}\right] \\ &= 2\ln(\frac{h}{\sqrt{\varepsilon_3}}) + 2\ln u - \ln\frac{1}{\sqrt{\varepsilon_1}} \\ &\quad - \ln\left[x_1 + \sqrt{x_1^2 + \frac{\varepsilon_1}{\varepsilon_3}h^2u^2}\right], \end{aligned}$$

and we can easily adapt the proof of Lemma 5.2 to reach the wanted conclusion. □

Propositions 3.7 and 3.8 use the following lemma, which is stated in the lecture notes of Kenneth Karlsen (2006) without proof.

Lemma 5.4 *Let* $u_n, v_n, u, v : \Omega \to \mathbb{R}$ *be measurable functions such that* $u_n \to u$ *in* $L^1(\Omega)$ *with* $\|u_n\|_\infty \le C$ *for all* n*. As* $n \to \infty$*, if* v_n *strongly (resp. weakly) converges to* v *in* $L^1(\Omega)$*, then* $u_n v_n$ *strongly (resp. weakly) converges to* uv *in* $L^1(\Omega)$*.*

Proof A proof for the case $u_n \to u$ a.e. is given in Lemma A.1 in Weber (2021), the same proof can be adapted to derive this lemma as well. □

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