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Liquid Crystals: Relaxed Energies, Dipoles, Singular Lines and Singular Points

M. GIAQUINTA - G. MODICA - J. SOUČEK

1. - Introduction

We discuss the relaxed functional of the liquid crystals energy. As a consequence we get the value of the energy of a dipole and we show concentration of the gradient on singular lines. In the last section we propose a modified energy for the minimizers of which both line and (non zero degree) point singularities are possible.

In [8], [9], [10], we have shown that, when dealing with variational problems for vector valued mappings, and especially for mappings with values into a manifold, the most natural setting is the one of *cartesian currents* there introduced. In the case of the energy of liquid crystals

$$\mathcal{E}(u) := \int_{\Omega} W(u(x), Du(x)) dx := \int_{\Omega} [\alpha |Du(x)|^2 + (k_1 - \alpha)(\operatorname{div} u(x))^2 + (k_2 - \alpha)(u(x) \cdot \operatorname{rot} u(x))^2 + (k_3 - \alpha)(u(x) \times \operatorname{rot} u(x))^2] dx$$

for mappings u from a bounded domain Ω of \mathbb{R}^3 of the type of ball into the unit sphere S^2 of \mathbb{R}^3 , $\alpha > 0$, $k_i > \alpha$, we were led to consider the parametric extension $\mathcal{E}(T)$ over the class $\operatorname{cart}^{2,1}(\Omega, S^2)$. The class $\operatorname{cart}^{2,1}(\Omega, S^2)$ is defined in [9], and can be characterized (by theorem 5.1 of [9]) as the class of 3-dimensional currents T in $\Omega \times S^2$, without boundary in $\Omega \times S^2$, for which there exist a unique function $u_T \in H^{1,2}(\Omega, S^2)$ and a unique 1-dimensional integer rectifiable current $L_T = \tau(\mathcal{L}, \theta, \zeta)$ in Ω such that

$$T = \llbracket G_{u_T} \rrbracket + L_T \times \llbracket S^2 \rrbracket$$

where $\llbracket G_{u_T} \rrbracket$ denotes the rectifiable current integration over the graph of u_T ,

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cf. [9]. Assuming for the sake of simplicity $\alpha = 1$, the parametric extension of $\mathcal{E}(u)$ is then given by

$$(1.1) \quad \mathcal{E}(T, \Omega) := \int_{\Omega} W(u_T(x), Du_T(x)) \, dx + 8\pi \Gamma(k_1, k_2, k_3) \mathbf{M}_{\Omega}(L_T),$$

where $\mathbf{M}_{\Omega}(L_T)$ denotes the mass of the current L_T in Ω , and

$$(1.2) \quad \Gamma(k_1, k_2, k_3) = \sqrt{k k_3} \int_0^1 \sqrt{1 + \gamma s^2} \, ds$$

where we have set

$$k = \min(k_1, k_2) \quad \text{and} \quad \gamma = \frac{k}{k_3} - 1.$$

Let φ be a boundary datum and assume that it is smooth, say $C^\infty(\partial\Omega, S^2)$. Suppose moreover that φ has degree zero on $\partial\Omega$, then we can think of φ as the restriction of a smooth function still denoted by φ and defined on some open set $\tilde{\Omega} \supset \Omega$. The Dirichlet problem amounts then to the problem of minimizing $\mathcal{E}(T, \tilde{\Omega})$ in the class

$$\text{cart}_{\varphi}^{2,1}(\tilde{\Omega}, S^2) := \left\{ T \in \text{cart}^{2,1}(\tilde{\Omega}, S^2) \mid T = \llbracket G_{\varphi} \rrbracket \text{ on } (\tilde{\Omega} \setminus \bar{\Omega}) \times S^2 \right\}.$$

The existence of a minimizer easily follows from the semicontinuity of $\mathcal{E}(T, \tilde{\Omega})$ with respect to the weak convergence in $\text{cart}^{2,1}(\tilde{\Omega}, S^2)$ and from the weak compactness of energy bounded sets in $\text{cart}^{2,1}(\tilde{\Omega}, S^2)$, cf. [9].

The main goal of this paper is to prove that $\mathcal{E}(T, \tilde{\Omega})$ is the relaxed functional of $\mathcal{E}(u)$ in $\text{cart}_{\varphi}^{2,1}(\tilde{\Omega}, S^2)$, i.e. that for all $T \in \text{cart}_{\varphi}^{2,1}(\tilde{\Omega}, S^2)$ there exists a sequence of smooth functions $\{u_k\}$, $u_k = \varphi$ on $\tilde{\Omega} \setminus \bar{\Omega}$, such that $\llbracket G_{u_k} \rrbracket \rightarrow T$ and

$$\mathcal{E}(T, \tilde{\Omega}) = \lim_{k \rightarrow \infty} \mathcal{E}(u_k);$$

consequently

$$(1.3) \quad \mathcal{E}(T, \tilde{\Omega}) := \inf \left\{ \liminf_{k \rightarrow \infty} \mathcal{E}(u_k) \mid u_k \text{ smooth, } u_k = \varphi \text{ on } \tilde{\Omega} \setminus \bar{\Omega}, \right. \\ \left. \sup_k \mathcal{E}(u_k) < +\infty, \llbracket G_{u_k} \rrbracket \rightarrow T \text{ in } \text{cart}^{2,1}(\tilde{\Omega}, S^2) \right\}.$$

THEOREM 1. *Let $T \in \text{cart}_{\varphi}^{2,1}(\tilde{\Omega}, S^2)$. Then there exists a sequence $\{u_k\}$ of smooth functions in $\tilde{\Omega}$, with $u_k = \varphi$ on $\tilde{\Omega} \setminus \bar{\Omega}$, such that*

$$\llbracket G_{u_k} \rrbracket \rightarrow T \quad \text{in } \text{cart}_{\varphi}^{2,1}(\tilde{\Omega}, S^2)$$

and

$$\int_{\tilde{\Omega}} W(u_k(x), Du_k(x)) dx \rightarrow \mathcal{E}(T, \tilde{\Omega}).$$

In proving this theorem, the discussion of the so-called *dipole problem* is relevant. Given two points a_{-1} and a_{+1} , we consider the class E of smooth mappings u from $\mathbb{R}^3 \setminus \{a_{+1}, a_{-1}\}$ into $S^2 \subset \mathbb{R}^3$ which map points outside some bounded region to some fixed point p of S^2 in \mathbb{R}^3 and which map small spheres around a_{-1}, a_{+1} into S^2 with degree respectively -1 and $+1$, i.e.

$$\deg(u, a_{-1}) = -1 \quad \deg(u, a_{+1}) = +1$$

compare [5]. The dipole problem for liquid crystals is then the problem of minimizing the energy $\mathcal{E}(u)$ in the class E . In the context of cartesian currents, this amounts to minimizing the parametric extension $\mathcal{E}(T)$ of $\mathcal{E}(u)$ in the class \tilde{E} of currents T in $\text{cart}_{\text{loc}}^{2,1}(\mathbb{R}^3 \setminus \{a_{+1}, a_{-1}\}, S^2)$ with $\partial T = [\{a_{-1}\} \times S^2] - [\{a_{+1}\} \times S^2]$, and T equals the graph $[[G_p]]$ of the constant map $x \in \mathbb{R}^3 \rightarrow p \in S^2$ outside some bounded region of \mathbb{R}^3 .

Consider the current $T_0 \in \text{cart}_{\text{loc}}^{2,1}(\mathbb{R}^3, S^2)$

$$T_0 := [[G_p]] + L \times [[S^2]]$$

where L is the 1-dimensional current integration over the oriented segment from a_{+1} to a_{-1} , to which we shall refer as to the *dipole* associated to the points $\{a_{-1}, a_{+1}\}$ and p at infinity. In section 3 we shall prove

THEOREM 2. *We have*

$$\inf_{u \in E} \mathcal{E}(u) = \mathcal{E}(T_0) = 8\pi \Gamma(k_1, k_2, k_3) |a_{+1} - a_{-1}|.$$

Moreover, there exists a sequence $\{u_k\}$ in E such that

$$[[G_{u_k}]] \rightarrow T_0 \quad \text{and} \quad \mathcal{E}([G_{u_k}]) \rightarrow \mathcal{E}(T_0)$$

as k tends to $+\infty$.

An immediate corollary of theorems 1 and 2 is that T_0 is a minimizer of $\mathcal{E}(T)$ in \tilde{E} , i.e.

$$\inf_{u \in E} \mathcal{E}(u) = \min_{T \in \tilde{E}} \mathcal{E}(T) = \mathcal{E}(T_0).$$

Coming back to the Dirichlet problem for $\mathcal{E}(T)$ in $\text{cart}_{\varphi}^{2,1}(\tilde{\Omega}, S^2)$ we point out, cf. [9], that our minimizers T , in contrast with $H^{1,2}(\Omega, S^2)$ minimizers, have in general line singularities but no point singularities with non-zero degrees. These line singularities show up, in the approximation by smooth maps, as lines where the “gradient” or more precisely the energy density, concentrates. This is stated in the next theorem.

THEOREM 3. Let $\{u_k\}$ be a sequence of smooth functions such that

$$\llbracket G_{u_k} \rrbracket \rightharpoonup T = \llbracket G_{u_T} \rrbracket + L_T \times \llbracket S^2 \rrbracket$$

in $\text{cart}_\varphi^{2,1}(\tilde{\Omega}, S^2)$ and $\mathcal{E}(u_k, \tilde{\Omega}) \rightarrow \mathcal{E}(T, \tilde{\Omega})$. Denote by $e(T)$ the energy measure of $\mathcal{E}(T)$, i.e.

$$e(T) = W(u_T(x), Du_T(x)) \mathcal{H}^3 + 8\pi \Gamma(k_1, k_2, k_3) \llbracket L_T \rrbracket$$

where $\llbracket L_T \rrbracket = \theta(x) \mathcal{H}^1 \llcorner L$, $L_T = \tau(L, \theta, \zeta)$. Then we have

- (i) $W(u_k(x), Du_k(x)) \mathcal{H}^3 \llcorner L \Omega$ converge as measures to $e(T)$.
- (ii) For all neighbourhoods U of $\text{spt } L$, $\{u_k\}$ converges to u strongly in $H^{1,2}(\tilde{\Omega} \setminus \bar{U}, S^2)$.

Although the geometry of the liquid crystal problem is different from the geometry of the problem of harmonic mappings, see section 2 for details, it is remarkable that the analytical setting is essentially equal, and in fact the proofs remind of the analogous proofs for the case of the Dirichlet energy, compare [10], but the basic idea and some important technical facts are different. The construction of the approximations depends on the constants k_1, k_2, k_3 and differs according to $k_1 \leq k_2$ or $k_1 \geq k_2$. The role played by the stereographic projection, in the case of the Dirichlet integral, is here taken by two new maps from \mathbb{R}^3 into S^2 which we call respectively *irrotational* and *solenoidal* dipoles. Moreover some extra work is needed, since we cannot construct approximations only for the dipole in which p is the *south pole* as in the case of Dirichlet's integral, because the energy $\mathcal{E}(u)$ is not invariant with respect to rotations in S^2 .

The proofs of theorems 1 and 2 will be given in section 4. Further remarks are contained in section 5 where we also propose a variant of the liquid crystals energy functional for the minimizers of which both point singularities of non-zero degree and line singularities are *a priori* possible.

2.- The energy functional and its parametric extension

The equilibrium configuration of a nematic liquid crystal in a domain Ω of \mathbb{R}^3 is described mathematically as a unitary vector field in Ω which minimizes the energy functional

$$\mathcal{E}(u) = \int_{\Omega} [\alpha |Du|^2 + (k_1 - \alpha)(\text{div } u)^2 + (k_2 - \alpha)(u \cdot \text{rot } u)^2 + (k_3 - \alpha)(u \times \text{rot } u)^2] dx \tag{2.1}$$

$\alpha > 0$, $k_i > \alpha$, under suitable boundary conditions, compare e.g. [6].

The integrand (2.1) has the invariance property

$$W(Qu, Q Du Q^T) = W(u, Du) \quad \forall Q \in O(3) \tag{2.2}$$

which makes $\mathcal{E}(u)$ well defined on the vector fields u in Ω . As usual, we represent any vectorfield $u(x)$ as a mapping $u : \Omega \subset \mathbb{R}_x^3 \rightarrow \mathbb{R}_y^3$ assuming that \mathbb{R}_x^3 and \mathbb{R}_y^3 are identified by a fixed isomorphism $i : \mathbb{R}_x^3 \rightarrow \mathbb{R}_y^3$. This way, the energy $\mathcal{E}(u)$ is defined for every map $u : \mathbb{R}_x^3 \rightarrow S^2 \subset \mathbb{R}_y^3$ by

$$\mathcal{E}(u) = \int_{\Omega} W(u(x), Du(x)) dx.$$

Assuming $\alpha = 1$, the integrand $W(n, G)$ is given, for any n in \mathbb{R}_y^3 and any linear map $G : \mathbb{R}_x^3 \rightarrow \mathbb{R}_y^3$, by

$$W(n, G) = |G|^2 + (k_1 - 1)(\text{trace } G)^2 + (k_2 - 1)(g \cdot n)^2 + (k_3 - 1)|g \times n|^2$$

where g is the axial vector of $G - G^T$, i.e. the vector defined by

$$(G - G^T)(v) = g \times v$$

or, in coordinates,

$$g_i = \varepsilon_{ijk} G_{jk}$$

ε_{ijk} being the components of the Levi-Civita tensor.

The next step is to regard $\mathcal{E}(u)$ as a functional defined on the graphs $G_u \subset \mathbb{R}^6$ of the mappings $u : \mathbb{R}_x^3 \rightarrow S^2 \subset \mathbb{R}_y^3$. This is done in [9], but for the reader's convenience and for future purposes we shall repeat here the main steps.

Let G be the matrix associated to the linear transformation G from \mathbb{R}_x^3 into \mathbb{R}_y^3 endowed with the standard basis (e_1, e_2, e_3) $(\varepsilon_1, \varepsilon_2, \varepsilon_3)$, where $\varepsilon_h = i(e_h)$. With the notation of [9], the tangent 3-vector $\xi \in \bigwedge_3 \mathbb{R}^6$ to the graph of the map $x \rightarrow Gx$ is given by

$$\xi = \frac{M(G)}{|M(G)|}$$

where

$$M(G) := (e_1 + G(e_1)) \wedge (e_2 + G(e_2)) \wedge (e_3 + G(e_3))$$

or in term of the minors of the matrix G

$$M(G) = \sum_{|\alpha|+|\beta|=n} \sigma(\alpha, \bar{\alpha}) M_{\beta\bar{\alpha}}(G) e^\alpha \wedge \varepsilon^\beta.$$

The decomposition $\mathbb{R}^6 = \mathbb{R}_x^3 \times \mathbb{R}_y^3$ splits $\bigwedge_3 \mathbb{R}^6$ as the direct sum

$$\bigwedge_3 \mathbb{R}^6 = \bigoplus_{k=0}^3 V_k$$

where

$$V_k = \bigwedge_{3-k} \mathbb{R}_x^3 \wedge \bigwedge_k \mathbb{R}_y^3$$

thus we can write every 3-vector $\xi \in \wedge_3 \mathbb{R}^6$ as

$$\xi = \sum_{k=0}^3 \xi_k \quad \xi_k \in V_k$$

and, in the same way,

$$M(G) = \sum_{k=0}^3 M_k(G).$$

More specifically one sees that

$$M_1(G) = \sum_{j=1}^3 (G_{j1} e_2 \wedge e_3 - G_{j2} e_1 \wedge e_3 + G_{j3} e_1 \wedge e_2) \wedge e_j.$$

If the matrix G has the vectors a, b, c as columns

$$G = \begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{pmatrix}$$

and satisfies $n^T \cdot G = 0$ for $n \in S^2$, one sees that

$$M_2(G) = \sum_{i=1}^3 D_i(n, G) e_i \wedge \varepsilon_n^{(2)}$$

where

$$\varepsilon_n^{(2)} = n_1 e_2 \wedge e_3 - n_2 e_1 \wedge e_3 + n_3 e_1 \wedge e_2$$

is the tangent 2-vector to $S^2 \subset \mathbb{R}_y^3$ at the point n , and $D_i(n, G)$ are the components of the vector

$$(2.3) \quad \mathbf{D}(n, G) = (n \cdot b \times c, n \cdot c \times a, n \cdot a \times b).$$

It is not difficult to see that in an intrinsic way $\mathbf{D}(n, G)$ can be defined by the relation

$$(2.4) \quad (\mathbf{D}(n, G), v \times w) = (n, Gv \times Gw) \quad \forall v, w \in \mathbb{R}_x^3.$$

Let now n be a point of S^2 . The polyconvex extension $F(n, \xi)$ of $W(n, G)$ is defined in [9] as the largest convex zero homogeneous minorant defined on $\{\xi \in \wedge_3 \mathbb{R}^6, \xi_{00} \geq 0\}$ and there it is proved that on simple vectors it has the following expression

$$F(n, \xi) = \begin{cases} W(n, G) & \text{if } \xi = \xi_{00} M(G), n^T \cdot G = 0, \xi_{00} > 0 \\ \Gamma(n, \xi_2) & \text{if } \xi_{00} = 0, \xi_1 = 0 \\ +\infty & \text{otherwise} \end{cases}$$

where

$$\Gamma(n, \xi_2) = \inf \{ W(n, G) \mid n^T \cdot G = 0, M_2(G) = \xi_2 \}$$

or equivalently, since ξ_2 is of the form $\xi_2 = t \wedge \varepsilon_n^{(2)}$,

$$\Gamma(n, t \wedge \varepsilon_n^{(2)}) = \inf \{ W(n, G) \mid n^T \cdot G = 0, \mathbf{D}(n, G) = t \}.$$

Moreover in [9] we found that

$$(2.5) \quad \Gamma(n, t \wedge \varepsilon_n^{(2)}) = 2\sqrt{k^2(t, n)^2 + kk_3(|t|^2 - (t, n)^2)}.$$

This way one sees that the functional $\mathcal{E}(u)$ extends to currents $T = \tau(\mathcal{M}, \theta, \xi)$ as

$$\mathcal{E}(T) = \int_{\mathcal{M}} F(y, \xi) \theta \, d\mathcal{H}^3(x, y);$$

therefore one sees, compare [9], that $\mathcal{E}(T)$ is finite on $\text{cart}^{2,1}(\Omega, S^2)$ and for

$$T = \llbracket G_{u_T} \rrbracket + L_T \times \llbracket S^2 \rrbracket,$$

$L_T = \tau(\mathcal{L}, \gamma, t)$ is given by

$$\mathcal{E}(T) = \int_{\Omega} W(u_T(x), Du_T(x)) \, dx + \int_{\mathcal{L} \times S^2} \gamma(x) \Gamma(n, t \wedge \varepsilon_n^{(2)}) \, d\mathcal{H}^1(x) \, d\mathcal{H}^2(n)$$

and, since

$$\int_{S^2} \Gamma(n, t \wedge \varepsilon_n^{(2)}) \, d\mathcal{H}^2(n) = 8\pi \Gamma(k_1, k_2, k_3)$$

we find the energy in (1.1) of the introduction.

3. - The dipole problem

In this section we prove theorem 2 of the introduction. This clearly amounts to proving: (i) $\forall u \in E, \mathcal{E}(u) \geq \mathcal{E}(T_0)$, (ii) there exists a sequence u_k in E such that $\llbracket G_{u_k} \rrbracket \rightarrow T_0$ and $\mathcal{E}(\llbracket G_{u_k} \rrbracket) \rightarrow \mathcal{E}(T_0)$. The proof of (i) relies on the coarea formula and Jensen's inequality, compare [1], [4], [5], while (ii) is proved by an explicit construction.

PROPOSITION 1. *We have*

$$\mathcal{E}(u) \geq \mathcal{E}(T_0)$$

for all $u \in E$.

PROOF. We may clearly assume that u is a map of class C^∞ in $\mathbb{R}^3 \setminus \{a_{-1}, a_{+1}\}$. By Sard's theorem, we know that almost every $n \in S^2$ is a regular value of u . Let n be any of such regular values but p . The implicit function theorem implies that $u^{-1}(n)$ is a collection of curves which either connect the points $a_{\pm 1}$ or are closed. Consider now the vector field

$$\mathbf{D}(x) := \mathbf{D}(u(x), Du(x))$$

which has been already considered in [5]. Since n is regular, we have

$$|\mathbf{D}(x)| = |M_2(Du(x))| > 0$$

moreover $\mathbf{D}(x)$ is tangent to the level line. In fact by (2.4) one deduces that

$$(\mathbf{D}(n, G), v \times t) = 0$$

for all t which are tangent to the level line $u(x) = n$, thus the conclusion follows as every normal vector to $u(x) = n$ can be written as $v \times t$ for some v . Also, since $\deg(u, a_{+1}) = 1$, $\deg(u, a_{-1}) = -1$, one can check that there exists at least one curve C_n in the level line $u(x) = n$ which, oriented by \mathbf{D} , goes from a_{+1} to a_{-1} .

From the definition of $\Gamma(n, \xi)$ in section 2, we now get that

$$\begin{aligned} W(u(x), Du(x)) &\geq \Gamma(u(x), M_2 Du(x)) \\ &= \Gamma\left(u(x), \frac{\mathbf{D}(x)}{|\mathbf{D}(x)|} \wedge \varepsilon_n^{(2)}\right) \cdot \|M_2(Du(x))\|; \end{aligned}$$

integrating over \mathbb{R}^3 and using the coarea formula, we then find

$$\begin{aligned} \mathcal{E}(u) &\geq \int_{\mathbb{R}^3} \Gamma\left(u(x), \frac{\mathbf{D}(x)}{|\mathbf{D}(x)|} \wedge \varepsilon_n^{(2)}\right) |M_2(Du(x))| dx \\ &\geq \int_{S^2} d\mathcal{H}^2(n) \int_{u(x)=n} \Gamma\left(n, \frac{\mathbf{D}(x)}{|\mathbf{D}(x)|} \wedge \varepsilon_n^{(2)}\right) d\mathcal{H}^1 \\ &\geq \int_{S^2} d\mathcal{H}^2(n) \int_{C_n} \Gamma\left(n, \frac{\mathbf{D}(x)}{|\mathbf{D}(x)|} \wedge \varepsilon_n^{(2)}\right) d\mathcal{H}^1. \end{aligned}$$

Since $\Gamma(n, \cdot \wedge \varepsilon_n^{(2)})$ is convex and 1-homogeneous, Jensen inequality yields

$$\mathcal{E}(u) \geq \int_{S^2} \Gamma\left(n, \int_{C_n} \frac{\mathbf{D}(x)}{|\mathbf{D}(x)|} d\mathcal{H}^1 \wedge \varepsilon_n^{(2)}\right) d\mathcal{H}^2(n)$$

and, as

$$\int_{C_n} \frac{\mathbf{D}(x)}{|\mathbf{D}(x)|} d\mathcal{H}^1 = a_{-1} - a_{+1}$$

we conclude with the inequality

$$\mathcal{E}(u) \geq \int_{S^2} \Gamma(n, (a_{-1} - a_{+1}) \wedge \varepsilon_n^{(2)}) d\mathcal{H}^2(n) = 8\pi \Gamma(k_1, k_2, k_3)$$

which is the claim.

q.e.d.

REMARK 1. In essentially the same way, but using the *slice* of \mathbb{R}^3 by the map u at points n in S^2 , compare [1], and the decomposition theorem for 1-dimensional currents [7] 4.2.25, one can show a slightly more general result: Suppose a_1, \dots, a_N are points in \mathbb{R}^3 and d_1, \dots, d_N are the prescribed degrees with $\sum_{i=1}^N d_i = 0$; then the infimum of the energies of smooth mappings from $\mathbb{R}^3 \setminus \{a_1, \dots, a_N\}$ to S^2 , which map points outside some bounded region in \mathbb{R}^3 to the point p of S^2 and which, for each i , satisfy $\deg(u, a_i) = d_i$, is not smaller than $8\pi \Gamma(k_1, k_2, k_3) \mathbf{M}(L)$, $\mathbf{M}(L)$ being the least mass of integral currents L in \mathbb{R}^3 with

$$\partial L = - \sum_{i=1}^N d_i \llbracket a_i \rrbracket$$

and, actually, it is equal, in view of theorem 1 of the introduction.

In order to prove this, one considers the *slice*

$$\langle \mathbb{R}^3, u, n \rangle = \tau(u^{-1}(n), \theta, \zeta)$$

compare [1], and one sees that

$$\partial \langle \mathbb{R}^3, u, n \rangle = - \sum_{i=1}^N d_i \llbracket a_i \rrbracket.$$

By the decomposition theorem [7], 4.2.25, one also has

$$\langle \mathbb{R}^3, u, n \rangle = \sum_{h=1}^{\infty} L_h, \quad \mathbf{M}(\langle \mathbb{R}^3, u, n \rangle) = \sum_{h=1}^{\infty} \mathbf{M}(L_h)$$

where L_h has multiplicity one and $\pm(\llbracket a_i \rrbracket - \llbracket a_j \rrbracket)$ as boundary. Thus, repeating the argument in the proof of proposition 1 for each L_i , the result follows.

The proof of the claim (ii) consists of two steps which are summarized in propositions 2 and 3 below. First we observe that because of the invariance

property (2.2) of the integrand of $\mathcal{E}(u)$, it is sufficient to construct an approximation of the dipole $T_0 = \llbracket G_p \rrbracket + L \times \llbracket S^2 \rrbracket$ only in the case that

$$L = \llbracket (0, 0, x_3) : 0 < x_3 < \ell \rrbracket$$

i.e. $a_{+1} = (0, 0, 0)$ and $a_{-1} = (0, 0, \ell)$, $\ell > 0$.

PROPOSITION 2. *There exists a function $\tilde{u}(x)$ from \mathbb{R}^2 into $S^2 \subset \mathbb{R}^3$ of class C^∞ such that*

- (i₁) $\tilde{u} = q$ at infinity, where q equals the “south pole” of $S^2 \subset \mathbb{R}^3$
- (i₂) \tilde{u} , seen as a map from S^2 into S^2 , has degree 1
- (i₃) if $\Omega := \mathbb{R}^2 \times (0, \ell)$ and $u : \Omega \rightarrow S^2$ is defined as

$$u(x_1, x_2, x_3) = \tilde{u}(x_1, x_2)$$

we have

$$\mathcal{E}(u) = 8\pi\ell \Gamma(k_1, k_2, k_3).$$

According to whether $k = \min(k_1, k_2)$ is k_1 or k_2 , we shall construct functions u that we call respectively the *irrotational* ($u \cdot \text{rot} u = 0$) and the *solenoidal* ($\text{div} u = 0$) dipoles with the properties in proposition 2.

In order to do that, we first observe that the energy of

$$T_0 := \llbracket G_q \rrbracket + L \times \llbracket S^2 \rrbracket$$

is

$$\mathcal{E}(T_0) = 2\ell \int_{S^2} \sqrt{k^2 n_3^2 + k k_3 (1 - n_3^2)} \, d\mathcal{H}^2(n)$$

where $n = (n_1, n_2, n_3) \in S^2$. Thus

$$\mathcal{E}(T_0) = 8\pi k \ell \int_0^1 \sqrt{\frac{k_3}{k} + \left(1 - \frac{k_3}{k}\right) z^2} \, dz$$

For future purposes, it is now convenient to set $z = \sqrt{1 - y^2}$ and write the energy of T_0 in the form

$$(3.1) \quad \mathcal{E}(T_0) = 8\pi k \ell \int_0^1 \frac{\sqrt{1 - \gamma y^2}}{\sqrt{1 - y^2}} y \, dy, \quad \gamma := 1 - \frac{k_3}{k}.$$

THE IRROTATIONAL DIPOLE. Assume $k = k_1$. We consider the maps $u : \Omega \rightarrow S^2$ of the form $u = (u_1, u_2, u_3)$

$$(3.2) \quad \begin{aligned} u_1(x) &= g(r) \frac{x_1}{r}, \\ u_2(x) &= g(r) \frac{x_2}{r}, \\ u_3(x) &= \text{sign}(1 - r) \sqrt{1 - g^2}, \end{aligned}$$

where

$$r = \sqrt{x_1^2 + x_2^2}$$

and

$$g : [0, +\infty[\rightarrow [0, 1]$$

is smooth and satisfies

$$(3.3) \quad \begin{aligned} g(0) &= 0, \quad g(1) = 1 \\ g(r) &\rightarrow 0 \quad \text{for } r \rightarrow +\infty \\ g'(r) &> 0 \quad \text{on } (0, 1) \\ g'(r) &< 0 \quad \text{on } (1, +\infty). \end{aligned}$$

Notice that $u \cdot \text{rot } u = 0$. For these mappings the energy is

$$\mathcal{E}(u) = 2\pi k\ell \int_0^{+\infty} \left[\frac{g^2}{r^2} + g'^2 \frac{1 - \gamma g^2}{1 - g^2} \right] r \, dr.$$

Taking into account that g is smooth and covers $(0, 1)$ twice, we can write in (3.1) $y = g(r)$ obtaining

$$\mathcal{E}(T_0) = 4\pi k\ell \int_0^\infty \frac{\sqrt{1 - \gamma g^2}}{\sqrt{1 - g^2}} \frac{g}{r} g' r \, dr$$

thus

$$\mathcal{E}(T_0) \leq 2\pi k\ell \int_0^\infty \left[\frac{g^2}{r^2} + g'^2 \frac{1 - \gamma g^2}{1 - g^2} \right] r \, dr$$

with equality if and only if

$$\frac{g^2}{r^2} = g'^2 \frac{1 - \gamma g^2}{1 - g^2}$$

that is, on account of (3.3), if and only if

$$(3.4) \quad g' = \text{sign}(1 - r) \frac{g}{r} \frac{\sqrt{1 - g^2}}{\sqrt{1 - \gamma g^2}}.$$

By a comparison argument, using in a neighbourhood of $r = 1$ the equation

$$g' = c \frac{g}{r} \sqrt{1 - g^2}, \quad c = \text{const.}$$

with solutions

$$g(r) = \frac{2r^c}{1 + r^{2c}}$$

and outside the equation

$$g' = c \frac{g}{r}$$

one easily sees that equation (3.4) is solvable under the conditions (3.3). In conclusion we can find a smooth *irrotational dipole* (3.2), (3.3), u such that

$$\mathcal{E}(u) = \mathcal{E}(T_0).$$

THE SOLENOIDAL DIPOLE. Assume $k = k_2$. We consider the maps $u : \Omega \rightarrow S^2$ of the form

$$(3.5) \quad \begin{aligned} u_1(x) &= g(r) \frac{x_2}{r}, \\ u_2(x) &= -g(r) \frac{x_1}{r}, \\ u_3(x) &= \text{sign}(1 - r) \sqrt{1 - g^2}, \end{aligned}$$

where $r = \sqrt{x_1^2 + x_2^2}$ and g satisfies the conditions (3.3) above. Notice that $\text{div } u = 0$. For these mappings the energy is given by

$$\mathcal{E}(u) = 2\pi k \ell \int_0^\infty \left[\frac{g^2}{r^2} (1 - \gamma g^2) + \frac{g'^2}{1 - g^2} \right] r \, dr$$

Similarly we find that

$$\mathcal{E}(T_0) \leq \mathcal{E}(u)$$

with equality if and only if

$$(3.6) \quad g' = \text{sign}(1 - r) \frac{g}{r} \sqrt{1 - g^2} \sqrt{1 - \gamma g^2}.$$

Again, by a similar comparison argument one then finds that (3.6) is solvable under the conditions (3.3). Hence we conclude that there exists a *solenoidal dipole* (3.5), (3.3), u such that

$$\mathcal{E}(u) = \mathcal{E}(T_0).$$

Clearly the previous constructions prove proposition 2.

We are now ready to state and prove proposition 3 which yields at once theorem 2 of the introduction.

PROPOSITION 3. *For every positive ε , there exists $u_\varepsilon \in E$ such that*

$$\mathcal{E}(u_\varepsilon) \leq \mathcal{E}(T_0) + \varepsilon.$$

Moreover, for ε tending to zero,

$$\llbracket G_{u_\varepsilon} \rrbracket \rightarrow T_0$$

in the sense of currents, and

$$\{x \in \mathbb{R}^3 : u_\varepsilon \neq p\} \downarrow \{(0, 0, x_3) : 0 < x_3 < \ell\}.$$

PROOF. Let \tilde{u} be the function in proposition 2. We can modify \tilde{u} near infinity, and more precisely outside a suitable ball $B_r \subset \mathbb{R}^2$, to the constant value $q =$ “south pole” changing the energy for less than ε , compare [5], [1]. This way we find $\tilde{v}_\varepsilon : \mathbb{R}^2 \rightarrow S^2$ with

$$\text{deg} \tilde{v}_\varepsilon = 1, \quad \tilde{v}_\varepsilon(x) = q \quad \forall x \in \mathbb{R}^2 \setminus B_r$$

and

$$\mathcal{E}(v_\varepsilon) \leq \mathcal{E}(T_0) + \varepsilon$$

where $v_\varepsilon(x_1, x_2, x_3) = \tilde{v}_\varepsilon(x_1, x_2)$. Let now p be any point in S^2 and let γ be a regular curve with finite length assumed to be parametrized by the arc length

$$\gamma : [0, t_\gamma(p)] \rightarrow S^2, \quad t_\gamma(p) = \text{length of } \gamma$$

and such that

$$\gamma(0) = q = \text{“south pole”}, \quad \gamma(t_\gamma(p)) = p.$$

For $R > r$ and $\rho^2 = x_1^2 + x_2^2$, set

$$(3.7) \quad \tilde{w}_\varepsilon = \begin{cases} \tilde{v}_\varepsilon(x_1, x_2) & \text{for } \rho < r \\ \gamma(t_\gamma(p) \theta_{r,R}(\rho)) & \text{for } r < \rho < R \\ p & \text{for } \rho > R \end{cases}$$

where

$$\theta_{r,R}(\rho) = \frac{\log \rho - \log r}{\log R - \log r}.$$

Clearly $\tilde{w}_\varepsilon \in C^{0,1}(\mathbb{R}^2, S^2)$, $\tilde{w}_\varepsilon = p$ outside B_R , $\text{deg} \tilde{w}_\varepsilon = 1$; moreover for

$$w_\varepsilon(x_1, x_2, x_3) := \tilde{w}_\varepsilon(x_1, x_2)$$

we have

$$\int_{B_r \times [0, \ell]} W(w_\varepsilon(x), Dw_\varepsilon(x)) \, dx = \int_{B_r \times [0, \ell]} W(v_\varepsilon(x), Dv_\varepsilon(x)) \, dx = \mathcal{E}(v_\varepsilon)$$

$$\int_{(B_R \setminus B_r) \times [0, \ell]} W(w_\varepsilon(x), Dw_\varepsilon(x)) \, dx \leq \text{const} \cdot \frac{t_\gamma^2(p)}{\log R - \log r};$$

hence, for R large enough,

$$\mathcal{E}(w_\varepsilon) \leq \mathcal{E}(T_0) + 2\varepsilon.$$

The proof can be now easily completed by applying the following simple observation, which we state as lemma 1, with $u = w_\varepsilon$, and δ sufficiently small.

LEMMA 1. *Let u be a function in $C^{0,1}(B_R \times (0, \ell), S^2)$ and let*

$$\phi_\delta(x_3) = \min(x_3, \ell - x_3, \delta).$$

Consider the map

$$\Phi_\delta(x_1, x_2, x_3) := (\phi_\delta(x_3)x_1, \phi_\delta(x_3)x_2, x_3)$$

and define

$$v_\delta(x) = u(\Phi_\delta^{-1}(x)).$$

Then we have

$$\int_{\Phi_\delta(B_R \times (0, \ell))} W(v_\delta(x), Dv_\delta(x)) \, dx$$

$$\leq \int_{B_R \times (0, \ell)} W(u(x), (u_{x_1}, u_{x_2}, 0)) \, dx + c \delta \int_{B_R \times (0, \ell)} |Du|^2 \, dx$$

where c is a constant depending on the Lipschitz constant of u .

We conclude this section with a proposition which will be used in the next section. Set

$$\Omega_\sigma := \left\{ (x_1, x_2, x_3) \mid \sqrt{x_1^2 + x_2^2} < \phi_\sigma(x_3) \right\}$$

$\phi_\sigma(x_3)$ being the function defined in lemma 1.

PROPOSITION 4. *Let $z(x_3)$ be a smooth function from \mathbb{R} into S^2 such that $z(x_3) = z(0)$ for $x_3 \leq 0$ and $z(x_3) = z(\ell)$ for $x_3 \geq \ell$. For all positive ε there exists*

a smooth function $u(x)$ from $\mathbb{R}^3 \setminus \{a_{-1}, a_{+1}\}$ into S^2 such that $\deg(u, a_{+1}) = +1$, $\deg(u, a_{-1}) = -1$, $u(x) = z(x_3)$ outside Ω_σ , and

$$\int_{\Omega_\sigma} W(u(x), Du(x)) dx \leq \mathcal{E}(T_0) + \varepsilon$$

provided σ is sufficiently small.

PROOF. We choose a regular curve which connects the south pole of S^2 to $z(0)$, $c(t) : [0, \tau_0] \rightarrow S^2$, $c(0) =$ “south pole”, $c(\tau_0) = z(0)$, and continue it as $c(\tau_0 + \tau) = z(\tau)$. Then we reparametrize $c(t)$ by its arc length and call it $\gamma(t)$. Setting

$$t_\gamma(z(x_3)) = \text{length of } c_{|[0, x_3]} ,$$

the construction (3.7), in the proof of proposition 3, yields for each x_3 a mapping \tilde{w}_ε depending on x_3 , $\tilde{w}_\varepsilon = \tilde{w}_\varepsilon^{(x_3)}$, which for $x_1^2 + x_2^2 > R^2$ has value $z(x_3)$, while for $x_1^2 + x_2^2 < r^2$ coincides with the function $\tilde{v}_\varepsilon(x_1, x_2)$ defined at the beginning of the proof of proposition 3. Since

$$\left| \frac{\partial \tilde{w}}{\partial x_3} \right| \leq \text{const} \cdot \left(1 + \frac{1}{r(\log R - \log r)} \right) |z'(x_3)| ,$$

the result easily follows applying lemma 1 to $u = w(x_1, x_2, x_3)$, with $w(x_1, x_2, x_3) = \tilde{w}_\varepsilon(x_1, x_2)$ and $\delta = \frac{\sigma}{R}$, and choosing σ sufficiently small.

q.e.d.

4. - The relaxed functional

In this section we shall prove theorems 1 and 3 of the introduction. In the proof we shall use without mention that the energy on a domain is small if and only if the Dirichlet energy is small in the same domain, since there are constants c_1, c_2 such that for all u and $G \subset \Omega$

$$c_1 \int_G |Du|^2 dx \leq \int_G W(u(x), Du(x)) dx \leq c_2 \int_G |Du|^2 dx.$$

The proof will be divided into two steps.

A. First assume that ∂L_T is rectifiable, i.e. that ∂L_T is a finite combination with integer coefficients of points in $\tilde{\Omega}$, and actually in Ω ,

$$\partial L_T = \sum_{i=1}^k \llbracket \hat{p}_i \rrbracket - \sum_{i=1}^k \llbracket \hat{n}_i \rrbracket$$

and that

$$u_T \in C^\infty \left(\tilde{\Omega} \setminus \bigcup_i \{p_i\} \cup \{n_i\} \right).$$

(i) *Approximation by polyhedral chains.* Using the approximation theorem of Federer [7], for all $\varepsilon > 0$ we can find a polyhedral chain P_ε and a diffeomorphism $\phi_\varepsilon : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ such that $\text{spt } P_\varepsilon$ is contained in an ε -neighbourhood U_ε of $\text{spt } L_T$, $\text{spt } P_\varepsilon \subset U_\varepsilon(\text{spt } L_T)$, and

$$\text{Lip } \phi_\varepsilon, \text{Lip } \phi_\varepsilon^{-1} \leq 1 + \varepsilon, \quad \phi_\varepsilon = \text{id on } \mathbb{R}^3 \setminus U_\varepsilon(\text{spt } L_T)$$

$$\mathbf{M}(P_\varepsilon - \phi_{\varepsilon\#}L_T) + \mathbf{M}(\partial P_\varepsilon - \phi_{\varepsilon\#}\partial L_T) < \varepsilon.$$

From the rectifiability of ∂P and ∂L , it follows that $\partial P_\varepsilon = \phi_{\varepsilon\#}\partial L_T$. Since $\text{spt } L_T$ is a finite number of points, we can also find a diffeomorphism

$$\psi_\varepsilon : \mathbb{R}^3 \rightarrow \mathbb{R}^3$$

such that

$$\psi_\varepsilon(\phi_\varepsilon(\Omega)) = \Omega,$$

$$\psi_\varepsilon = \phi_\varepsilon = \text{id}_{\partial\Omega},$$

$$\psi_\varepsilon = \text{id on spt } \partial P_\varepsilon = \text{spt } \phi_{\varepsilon\#}\partial L_T$$

and

$$\text{Lip } \psi_\varepsilon, \text{Lip } \psi_\varepsilon^{-1} \leq 1 + c\varepsilon.$$

If we now move the vertices of P_ε which are not in ∂P_ε by ψ_ε , we finally find a new polyhedral chain \tilde{P}_ε with $\text{spt } \tilde{P}_\varepsilon \subset \Omega$, $\text{spt } \tilde{P}_\varepsilon \subset U_{c\varepsilon}(\text{spt } P_\varepsilon)$, $\partial \tilde{P}_\varepsilon = \partial P_\varepsilon$ and clearly the currents

$$T_\varepsilon := \llbracket G_{u_\varepsilon} \rrbracket + \tilde{P}_\varepsilon \times \llbracket S^2 \rrbracket, \quad u_\varepsilon(x) := u_T(\psi_\varepsilon(\phi_\varepsilon(x)))$$

converge weakly for $\varepsilon \rightarrow 0$ to T and $\mathcal{E}(T_\varepsilon, \tilde{\Omega}) \rightarrow \mathcal{E}(T, \tilde{\Omega})$.

(ii) *Approximation by non autointersecting and density 1 polyhedral chains.* Let $T \in \llbracket G_{u_T} \rrbracket + P \times \llbracket S^2 \rrbracket \in \text{cart}_{\varphi}^{2,1}(\tilde{\Omega}, S^2)$, P polyhedral, $\text{spt } P \subset \Omega$ and $u_T \in C^\infty(\tilde{\Omega} \setminus \text{spt } \partial P)$. We have

$$P = \sum_i \llbracket (n_i, p_i) \rrbracket$$

where (n_i, p_i) is the oriented segment joining n_i to p_i , (the points n_i , respectively p_i , are not in general distinct). We claim that we can reorder the indexes i in such a way that if $p_i \notin \partial P$ then $p_i = n_{i+1}$. In fact, if $n_1 \in \partial P$ and there exists some $n_{\tilde{1}} = p_1$, we rename n_i as \tilde{n}_1 and we consider $(\tilde{n}_1, \tilde{p}_1)$, $\tilde{p}_1 := p_{\tilde{1}}$. If there exists $n_i \neq \tilde{n}_1$ with $n_i = \tilde{p}_1$, we rename n_i as \tilde{n}_2 and we continue this way until we are able to find points n_i different from the ones already chosen; this

process clearly finishes in a finite number of steps, and the final \tilde{p}_k we find must obviously belong to ∂P . Once the construction has been carried out for all $n_i \in \partial P$, we start with any n_i (if any is left) and we repeat the construction until we come back to some $p_k = n_i$ (observe that this must happen since we have already used all $n_i \in \partial P$, thus all $p_i \in \partial P$) and we continue this way. Observe that as a result of our construction on each point of ∂P chains either start or finish. Clearly we can now slightly move the $p_k = n_{k+1}$, which do not belong to ∂P , in such a way that the new $\bar{p}_k = \bar{n}_{k+1}$ belong to Ω and are distinct, the segments (\bar{n}_k, \bar{p}_k) do not intersect in $\Omega \setminus \text{spt } \partial P$ and finally

$$\tilde{P} := \sum_k \llbracket (\bar{n}_k, \bar{p}_k) \rrbracket \subset U_\varepsilon(\text{spt } P).$$

We therefore conclude that we can find a sequence of finite polyhedral lines $P^{(k)}$ (which are either closed or start and finish on ∂P), without autointersections, such that $\partial P^{(k)} = \partial P$, $P^{(k)} \rightarrow P$ and $\mathbf{M}(P^{(k)}) \rightarrow \mathbf{M}(P)$. We emphasize that, on each point of ∂P , lines of $P^{(k)}$ either all start or all finish.

(iii) *Adding small dipoles.* Let $T = \llbracket G_u \rrbracket + P \times \llbracket S^2 \rrbracket \in \text{cart}_\varphi^{2,1}(\tilde{\Omega}, S^2)$ where P is a polyhedral chain as in the conclusion of (ii) and $u_T \in C^\infty(\tilde{\Omega} \setminus \text{spt } \partial P)$. Let $x_0 \in \Omega \setminus \text{spt } \partial P$ and ε be a positive small number. We claim that for all x_1 in $B(x_0, \delta)$, δ small, there exists $v \in C^\infty(\tilde{\Omega} \setminus (\text{spt } \partial P \cup \{x_0\} \cup \{x_1\}))$, $v = u$ on $\Omega \setminus B(x_0, \delta)$, such that

$$\int_{B(x_0, \delta)} W(v(x), Dv(x)) \, dx \leq \int_{B(x_0, \delta)} W(u(x), Du(x)) + \varepsilon$$

$$\text{deg}(v, x_0) = -\text{deg}(v, x_1) = 1 .$$

In fact, if δ is sufficiently small, the oscillation of u on $\partial B(x_0, \delta)$ is small, thus we can extend smoothly u to $B(x_0, \delta)$ as \tilde{u} with $\tilde{u} = \text{constant}$ on $B(x_0, \delta/2)$ and with $\int_{B(x_0, \delta)} |D\tilde{u}|^2 \, dx$ small. Applying to $B(x_0, \delta/2)$ the dipole construction of [5], or proposition 4 of section 3, the claim follows.

(iv) *Approximating large dipoles.* Let $T = \llbracket G_u \rrbracket + P \times \llbracket S^2 \rrbracket \in \text{cart}_\varphi^{2,1}(\tilde{\Omega}, S^2)$ where P is a polyhedral chain as in the conclusion (ii) and $u \in C^\infty(\tilde{\Omega} \setminus \text{spt } \partial P)$. Let $S = \llbracket n_i, p_i \rrbracket$ be one of the segments of P . By choosing a suitable system of coordinates in \mathbb{R}_x^3 and accordingly in \mathbb{R}_y^3 , so that the energy remains invariant, we may assume that

$$S = \{(0, 0, x_3) \mid -\mu < x_3 < \ell + \mu\}$$

where $\mu > 0$ is sufficiently small. Applying proposition 4 section 3, we can find for σ sufficiently small

$$\Omega_\sigma = \{(x_1, x_2, x_3) \mid x_1^2 + x_2^2 < \phi_\sigma^2(x_3), 0 < x_3 < \ell\}$$

and \bar{u} such that

$$\bar{u}(x) = \begin{cases} u(x) & \text{in } \Omega \setminus \tilde{\Omega}_\sigma \\ u\left(\frac{2\rho-2\phi_\delta(x_3)}{\rho}x_1, \frac{2\rho-2\phi_\delta(x_3)}{\rho}x_2, x_3\right) & \text{in } \tilde{\Omega}_\sigma \setminus \Omega_\sigma \end{cases}$$

$\rho = \sqrt{x_1^2 + x_2^2}$ and

$$\tilde{\Omega}_\sigma = \{(x_1, x_2, x_3) \mid x_1^2 + x_2^2 < 4\phi_\sigma^2(x_3), 0 < x_3 < \ell\}$$

such that

$$\int_{\tilde{\Omega}_\sigma} W(\bar{u}(x), D\bar{u}(x)) \, dx \leq 8\pi \Gamma(k_1, k_2, k_3) \mathbf{M}(S) + \varepsilon.$$

Coming back to the original coordinates, consider now the current

$$\tilde{T} = \llbracket G_{\bar{u}} \rrbracket + \tilde{P} \times \llbracket S^2 \rrbracket$$

where \tilde{P} is obtained by replacing S with the two small segments, one starting in n_i and ending in a point near n_i on S and the other starting in a point on S near p_i and ending in p_i . Then it is easily seen that $\tilde{T} \in \text{cart}_{\varphi}^{2,1}(\tilde{\Omega}, S^2)$ and

$$\mathcal{E}(\tilde{T}) \leq \mathcal{E}(T) + \varepsilon.$$

Repeating the same argument on each segment S of P , we conclude that there exists a current $\hat{T} \in \text{cart}_{\varphi}^{2,1}(\tilde{\Omega}, S^2)$

$$\hat{T} = \llbracket G_{\hat{u}} \rrbracket + \hat{P} \times \llbracket S^2 \rrbracket$$

such that

$$\hat{P} = \sum_{i=1}^N \llbracket \hat{n}_i, \hat{p}_i \rrbracket, \quad \mathbf{M}(\hat{P}) \text{ small}$$

$$\hat{u} \in C^\infty(\tilde{\Omega} \setminus \cup_i \{\hat{n}_i, \hat{p}_i\}, S^2)$$

and finally

$$\mathcal{E}(\hat{T}) \leq \mathcal{E}(T) + \varepsilon.$$

Since the mass of each $\llbracket \hat{n}_i, \hat{p}_i \rrbracket$ is small, we can find a finite number of small balls B_i such that $\text{deg}(\hat{u}, \partial B_i) = 0$ and $\mathbf{M}(\hat{P} \llcorner B_i)$ is small. Then applying theorem 2 of [2] or theorem 2 of [10], the proof of our theorem is completed under the extra assumption A.

B. Let $T = \llbracket G_u \rrbracket + L \times \llbracket S^2 \rrbracket$ be a generic element of $\text{cart}_{\varphi}^{2,1}(\tilde{\Omega}, S^2)$. We claim that T can be approximated weakly and in energy by a sequence of currents satisfying assumption A. This of course concludes the proof of our theorem.

The proof of the above claim is the same as in [10] pp.501-503. Thus we shall omit it.

q.e.d.

We conclude this section by proving theorem 3. Let $\{u_k\}$ be a sequence of smooth functions such that

$$\llbracket G_{u_k} \rrbracket \rightarrow \llbracket G_u \rrbracket + L \times \llbracket S^2 \rrbracket \quad \text{in } \text{cart}_\varphi^{2,1}(\tilde{\Omega}, S^2)$$

and $\mathcal{E}(u_k, \tilde{\Omega}) \rightarrow \mathcal{E}(T, \tilde{\Omega})$. Passing to a subsequence we have

$$e(\llbracket G_{u_k} \rrbracket) \rightarrow \mu_0$$

in the sense of measures. For all $\psi \in C_0^0(\tilde{\Omega})$, $\psi \geq 0$, consider the functional

$$\mathcal{F}(T) := \int \psi(x) \, de(T)$$

From [9] we know that \mathcal{F} is lower semicontinuous with respect to the convergence in $\text{cart}_\varphi^{2,1}(\tilde{\Omega}, S^2)$, thus we conclude that

$$e(T)(\psi) = \mathcal{F}(T) \leq \liminf_{k \rightarrow \infty} \mathcal{F}(u_k) = \mu_0(\psi)$$

i.e. $e(T) \leq \mu_0$. As $\mathcal{E}(u_k, \tilde{\Omega}) \rightarrow \mathcal{E}(T, \tilde{\Omega})$ we then get $(\mu_0 - e(T))(\tilde{\Omega}) = 0$, i.e. $e(T) = \mu_0$. This yields (i) of theorem 3 of the introduction. In order to prove the claim (ii), we observe that for all neighbourhoods U of $\text{spt } L$, we have

$$u_k \rightarrow u \quad \text{in } H^{1,2}(\tilde{\Omega} \setminus \bar{U}, S^2)$$

$$\int_{\tilde{\Omega} \setminus U} W(u_k(x), Du_k(x)) \, dx \rightarrow \int_{\tilde{\Omega} \setminus U} W(u(x), Du(x)) \, dx.$$

As W is strictly convex with respect to Du , a known theorem of Reshetnyak, [14] p. 329, applied to our functional seen in the product space $(\tilde{\Omega} \setminus \bar{U}) \times S^2$, compare [8] p. 137, implies that

$$\int_{\tilde{\Omega} \setminus U} |Du_k|^2 \, dx \rightarrow \int_{\tilde{\Omega} \setminus U} |Du|^2 \, dx$$

and this clearly implies strong convergence in $H^{1,2}(\tilde{\Omega} \setminus \bar{U}, S^2)$.

q.e.d.

5. Final remarks

In this final section we shall deal with two more questions. The first one concerns the *relaxed energy in* $H_\varphi^{1,2}(\tilde{\Omega}, S^2)$. The second question concerns the possibility of finding a unified approach to the problem of minimizing the energy of liquid crystals in $H_\varphi^{1,2}(\Omega, S^2)$ and $\text{cart}_\varphi^{2,1}(\Omega, S^2)$ to allow the possible occurrence of line and (non zero degree) point singularities for the minimizers.

Let φ be a given smooth function in $\tilde{\Omega} \supset \Omega$. For all u in

$$H_\varphi^{1,2}(\tilde{\Omega}, S^2) := \left\{ u \in H^{1,2}(\tilde{\Omega}, S^2) : u = \varphi \text{ in } \tilde{\Omega} \setminus \Omega \right\}$$

we consider the class

$$[u] := \left\{ T = \llbracket G_{u_T} \rrbracket + L_T \times \llbracket S^2 \rrbracket \in \text{cart}_\varphi^{2,1}(\Omega, S^2) : u_T = u \right\}$$

and we denote by T_u the minimizer of $\mathcal{E}(T)$ in $[u]$ which clearly exists; also, we consider the new functional $E(u)$ defined in $H^{1,2}(\tilde{\Omega}, S^2)$ as

$$E(u) := \mathcal{E}(T_u) = \int_{\Omega} W(u(x), Du(x)) dx + 8\pi \Gamma(k_1, k_2, k_3) \mathbf{M}(L_{T_u}).$$

In [10] we have proved that

$$L(u) := \frac{1}{4\pi} \sup_{\substack{\xi: \Omega \rightarrow \mathbb{R} \\ \|D\xi\|_\infty \leq 1}} \left\{ \int_{\Omega} \mathbf{D}(u, Du) \cdot D\xi dx - \int_{\partial\Omega} \mathbf{D}(u, Du) \cdot n \xi d\mathcal{H}^2 \right\} \\ = \mathbf{M}(T_u).$$

Thus we can express $E(u)$ in terms of u as

$$E(u) = \int_{\Omega} W(u(x), Du(x)) dx + 2 \Gamma(k_1, k_2, k_3) L(u) .$$

The semicontinuity of \mathcal{E} obviously yields that $E(u)$ is lower semicontinuous with respect to the weak convergence in $H_\varphi^{1,2}(\tilde{\Omega}, S^2)$. Moreover, our previous results yield at once that for all $u \in H_\varphi^{1,2}(\tilde{\Omega}, S^2)$ there exists a sequence $\{u_k\} \subset C^1(\tilde{\Omega}, S^2)$, $u_k = \varphi$ on $\tilde{\Omega} \setminus \bar{\Omega}$, $u_k \rightharpoonup u$ in $H_\varphi^{1,2}(\tilde{\Omega}, S^2)$, such that

$$\int_{\tilde{\Omega}} W(u_k(x), Du_k(x)) dx \rightarrow E(u).$$

Thus we see that $E(u)$ is the *relaxed functional of* $\mathcal{E}(u)$ in $H_\varphi^{1,2}(\tilde{\Omega}, S^2)$. This extends previous results obtained in [3] for the Dirichlet's energy to the liquid crystal energy.

Let us now discuss our second question. We consider the class of currents T in $\Omega \times S^2$ of the type

$$T = \llbracket G_u \rrbracket + L \times \llbracket S^2 \rrbracket$$

satisfying

$$\|T\|_{Cf^{2,1}(\Omega, S^2)} := \left(\int_{\Omega} |Du|^2 dx \right)^{1/2} + \mathbf{M}(L) + \mathbf{M}(\partial T) < +\infty$$

but we do not require that they are boundaryless in $\Omega \times S^2$. We denote this class by $Cf^{2,1}(\Omega, S^2)$, as cartesian currents with fractures.

PROPOSITION 5. *We have*

- (i) *For any $u \in H^{1,2}(\Omega, S^2)$ there exists a zero dimensional current Z_u in Ω such that*

$$\partial \llbracket G_u \rrbracket \llcorner (\Omega \times S^2) = Z_u \times \llbracket S^2 \rrbracket$$

- (ii) *If $T_k \in Cf^{2,1}(\Omega, S^2)$, $T_k \rightharpoonup T$ in the sense of currents, and*

$$(5.1) \quad \sup_k \|T_k\|_{Cf^{2,1}(\Omega, S^2)} < +\infty$$

then T belongs to $Cf^{2,1}(\Omega, S^2)$.

PROOF. (i) By a result in [2], there exists a sequence $\{u_k\} \in C^\infty(\Omega, S^2)$, $u_k \rightharpoonup u$ in $H^{1,2}(\Omega, S^2)$; clearly the sequence $\llbracket G_{u_k} \rrbracket$ is equibounded in $cart^{2,1}(\Omega, S^2)$, thus by theorem 1 section 5 of [9] we have, passing to a subsequence,

$$\llbracket G_{u_k} \rrbracket \rightharpoonup T = \llbracket G_{u_T} \rrbracket + L_T \times \llbracket S^2 \rrbracket \quad \text{in } cart^{2,1}(\Omega, S^2)$$

and $u_T = u$. Then the claim follows by taking $Z = -\partial L_T$, since $\partial T = 0$.

- (ii) Let $T_k = \llbracket G_{u_k} \rrbracket + L_k \times \llbracket S^2 \rrbracket$. By (i) we have

$$\partial T_k = Z_k \times \llbracket S^2 \rrbracket$$

and by (5.1)

$$\sup_k \mathbf{M}(Z_k) < +\infty$$

Thus, passing to a subsequence, Z_k converges weakly to some zero dimensional current Z with $\mathbf{M}(Z) < +\infty$, consequently Z is a finite sum of current integration over points $\{a_i\}$ in Ω . Clearly $T \llcorner (\Omega \setminus \cup\{a_i\}) \times \llbracket S^2 \rrbracket$ belong to $cart^{2,1}(\Omega \setminus \cup\{a_i\}, S^2)$, hence $T \in Cf^{2,1}(\Omega, S^2)$.

q.e.d.

We introduce now a modified energy for the liquid crystals as

$$\begin{aligned} \mathcal{E}_\gamma(T) &:= \mathcal{E}(T) + \gamma \mathbf{M}(\partial T) \\ &= \int W(u(x), Du(x)) \, dx + 8\pi \Gamma(k_1, k_2, k_3) \mathbf{M}(L) + \gamma \mathbf{M}(\partial T) \end{aligned}$$

for all T in $Cf^{2,1}(\Omega, S^2)$, where γ is a positive constant. Choose $\tilde{\Omega} \supset \supset \Omega$, fix a smooth function ϕ in $\tilde{\Omega} \setminus \Omega$, and consider the problem of minimizing $\mathcal{E}_\gamma(T)$ in the class

$$Cf_\phi^{2,1}(\tilde{\Omega}, S^2) = \left\{ T \in Cf^{2,1}(\tilde{\Omega}, S^2) : T \llcorner (\tilde{\Omega} \setminus \Omega) \times S^2 = \llbracket G_\phi \rrbracket \right\}.$$

Since $\mathcal{E}(T)$ and consequently $\mathcal{E}_\gamma(T)$ is lower semicontinuous with respect to the convergence of currents, compare [8], and \mathcal{E}_γ is coercive with respect to $\|\cdot\|_{Cf^{2,1}(\tilde{\Omega}, S^2)}$, we conclude at once with

PROPOSITION 6. *For all positive γ there exists a minimizer of $\mathcal{E}_\gamma(T)$ in $Cf^{2,1}(\tilde{\Omega}, S^2)$.*

We point out that $\phi|_{\partial\Omega}$ need not have degree zero, and that in general $\partial(T \llcorner (\tilde{\Omega} \times S^2)) \neq -\partial \llbracket G_\phi \rrbracket$ for $T \in Cf_\phi^{2,1}(\tilde{\Omega}, S^2)$; thus the boundary datum is taken in the sense of a strong anchorage, but not in the sense of the boundary of currents; in principle we only have $u_T = \phi$ on $\partial\Omega$ in the sense of the traces in $H^{1,2}(\Omega, S^2)$.

Secondly, the minimizer T in proposition 6 has in general non zero boundary in $\tilde{\Omega} \times \llbracket S^2 \rrbracket$, and actually the gap phenomenon, observed by Hardt and Lin [13], shows that, for suitable boundary data ϕ (even with zero degree on $\partial\Omega$) and for γ not too large, the minimizer T must have non-zero boundary in $\tilde{\Omega} \times \llbracket S^2 \rrbracket$. The boundary

$$\partial T \llcorner \tilde{\Omega} \times S^2 = \sum_{i=1}^N d_i \llbracket \{a_i\} \times S^2 \rrbracket,$$

$d_i \in \mathbb{Z}$, can be interpreted as a fracture in the configuration of the liquid crystal, and the term $\gamma \mathbf{M}(\partial T)$ as the amount of energy needed or payed in order to produce the fracture, compare [9].

Notice moreover that the minimizers T of \mathcal{E}_γ show interesting features. In fact for T it is not convenient to create two fractures with opposite degrees one close to the other, as the corresponding dipole would contribute less to the energy, while it is not convenient to create a long dipole as the creation of two fractures would decrease the energy. Concluding, in this model, both line and point singularities may appear, point singularities being interpreted as point fractures of the crystal, while line singularities show up as lines where the “gradient” concentrates.

Finally we observe that for $\gamma = 0$, our variational problem reduces simply to minimizing the liquid crystal energy in $H^{1,2}(\Omega, S^2)$, [12], while for $\gamma = +\infty$ it reduces to minimizing the relaxed functional in $\text{cart}^{2,1}(\Omega, S^2)$.

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