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Minimizing Oseen-Frank energy for nematic liquid crystals: algorithms and numerical results

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ABSTRACT. – We propose a family of new algorithms for computing stable equilibrium configurations of nematic liquid crystals, using the Oseen-Frank energy and with constants varying in the full physical range. These algorithms, first given in a continuous setting, are then numerically implemented and the stability of the hedgehog solution with respect to variations of each of the constants is discussed. The calculations presented show that the classical relation, first given by Hélein, does not seem to be optimal thus leading to new issues. The paper ends with an appendix showing the ellipticity of the Euler equations related to the problem. Thanks to the efficiency of the algorithms, these computations can be performed on a workstation.

Key words: Nematic liquid crystals, non convex optimization, conjugate gradients, nonlinear elliptic problems.

RÉSUMÉ. – Nous proposons dans cet article une famille d'algorithmes pour le calcul de configurations d'équilibre stables de cristaux liquides nématiques en utilisant le modèle d'Oseen-Frank où les constantes peuvent être arbitrairement choisies. Ces algorithmes sont d'abord étudiés dans un cadre abstrait puis implantés numériquement. Le principal cas-test utilisé est celui de la stabilité de la solution dite « hérisson » en fonction des valeurs des constantes du modèle. On montre numériquement que la relation donnée par Hélein liant la stabilité aux valeurs de ces constantes, ne semble pas optimale. À la fin de l'article, on prouve l'ellipticité des équations d'Euler liées au problème.

Mots clés : Cristaux liquides nématiques, optimisation non convexe, gradient conjugué, problèmes elliptiques non-linéaires.

Contents

1. INTRODUCTION

Local minima of the Oseen-Frank energy

$$\mathcal{E}(u) = \int_{\Omega} \mathcal{W}(u, \nabla u) dx, \tag{1.1}$$

where

$$\mathcal{W}(u, \nabla u) = \sum_{i,j,k,l} a_{ijkl}(u) \frac{\partial u_i}{\partial x_j} \frac{\partial u_k}{\partial x_l} dx, \tag{1.2}$$

describe equilibrium configurations of a nematic liquid crystal. The vector field u, defined on Ω (the bounded region in $\mathbb{R}^3$ occupied by the liquid crystal), takes its values in the sphere $S^2 = \{v \in \mathbb{R}^3, v_1^2 + v_2^2 + v_3^2 = 1\}$ and we will assume a strong anchoring condition on $\partial\Omega$ the boundary of Ω. Namely we presume that

$$u(x) = \varphi(x) \quad \text{for } x \in \partial\Omega, \tag{1.3}$$

for a given mapping φ from $\partial\Omega$ into S^2. Physical considerations (see e.g. de Gennes [14]) lead then to the following expression for $\mathcal{W}$:

$$\begin{aligned} 2\mathcal{W}(u, \nabla u) =& K_1(\text{ div } u)^2 + K_2(u \cdot \text{curl } u)^2 + K_3|u \times \text{curl } u| \\ &+ (K_2 + K_4)(tr(\nabla u)^2 - (\text{ div } u)^2) \end{aligned} \tag{1.4}$$

where K_1, K_2 and K_3 are positive constants. For usual nematic liquid crystals, these constants which depend heavily on the temperature, are not equal, but are nevertheless of the same order of magnitude (see Table 1 for a few examples). Indeed, in a nematic liquid crystal, three types of deformation can occur: splay ($\text{div}(u) \neq 0$), bend ($\text{curl}(u) \perp u$) and twist ($\text{curl}(u) \parallel u$) as described in Figure 1 (Table 1 and Figure 1 are extracted from [14]).

Our aim in this work is to study from the numerical point of view the minimization problem

$$\underset{\substack{u:\Omega \to S^2 \\ u=\varphi \text{ on } \partial\Omega}}{\text{Min}} \quad \mathcal{E}(u), \tag{1.5}$$

and we are interested in finding either the solution(s) to (1.5) or local minimizers, which are functions u which minimize the energy $\mathcal{E}(v)$ for v in a neighborhood (for a suitable topology) of u.

TABLE 1

Elastic constants for p-azoxyanisole (PAA) and N-(p-methoxybenzylindene)-p-butylaniline (MBBA).

Temp. (°C)	K_1 (dynes)	K_2 (dynes)	K_3 (dynes)	Material
120	$5.0\ 10^{-7}$	$3.8\ 10^{-7}$	$10.1\ 10^{-7}$	PAA
125	$4.5\ 10^{-7}$	$2.9\ 10^{-7}$	$9.5\ 10^{-7}$	PAA
129	$3.85\ 10^{-7}$	$2.4\ 10^{-7}$	$7.7\ 10^{-7}$	PAA
22	$5.3\ 10^{-7}$	$2.2\ 10^{-7}$	$7.45\ 10^{-7}$	MBBA

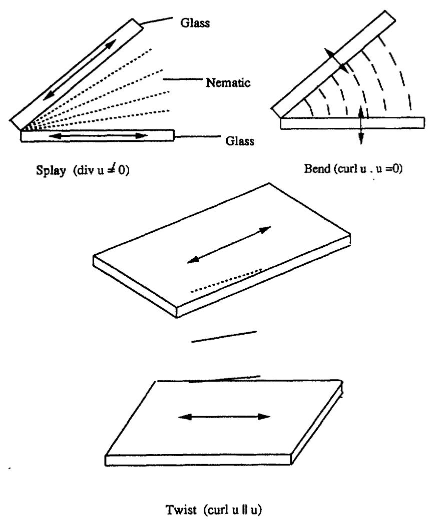

Fig. 1. – Deformations occurring in nematics.

In the next Section we give a brief survey of some of the prior work on this problem with particular emphasis on the results which are related with our objectives. In Section 3 we introduce a family of algorithms that produce a sequence $(u_n)_{n\in\mathbb{N}}$ of functions from $\overline{\Omega}$ into S^2 satisfying (1.3) and such that $\mathcal{E}(u_{n+1}) \leqslant \mathcal{E}(u_n)$, *i.e.*, of functions with decreasing energy. Section 4 is then devoted to the discretization of these algorithms. In Section 5 we describe the numerical results obtained and compare the performance of some of the algorithms. In view of these results we draw some conclusions about (1.5) in Section 6 and also indicate further investigations we intend to carry out in the future. Finally, a technical appendix about the ellipticity of the Euler-Lagrange equations associated to problem (1.5) ends the paper.

2. A BRIEF SURVEY OF CONTINUOUS RESULTS

2.1. Some analytical facts

The first observation (due independently to Oseen and Ericksen) is that the value of K_4 (see (1.4)) does not contribute to (1.5). More precisely

$$\int_\Omega (\mathrm{tr}(\nabla u)^2 - (\mathrm{div}\ u)^2)dx \tag{2.1}$$

depends only on the value of the trace of u on $\partial\Omega$. This is due to the following two facts: first

$$\mathrm{tr}(\nabla u)^2 - (\mathrm{div}\ u)^2 = \mathrm{div}\ ((u \cdot \nabla)u - (\mathrm{div}\ u)u) \tag{2.2}$$

and second, the first order differential operator D_t defined by

$$D_t v = \nabla v - \nu \otimes \frac{\partial v}{\partial \nu} \tag{2.3}$$

where ν stands for the outward normal, is a differential operator on $\partial\Omega$, which is to say it involves only tangential derivatives. Hence by the divergence theorem

$$\begin{aligned}\int_\Omega (\mathrm{tr}(\nabla u)^2 - (\mathrm{div}\ u)^2)dx &= \int_{\partial\Omega} (u.\nabla u - (\mathrm{div}\ u)u).\nu d\sigma \\ &= \int_{\partial\Omega} (D_t u : u \otimes \nu - \mathrm{tr}(D_t u)u.\nu)d\sigma. \end{aligned} \tag{2.4}$$

Therefore using (1.3), we obtain

$$\int_\Omega (\mathrm{tr}(\nabla u)^2 - (\mathrm{div}\ u)^2)dx = \int_{\partial\Omega} (D_t \varphi : \varphi \otimes \nu - \mathrm{tr}(D_t \varphi)\varphi.\nu)d\sigma. \tag{2.5}$$

This shows that in studying problems of the form in (1.5), one can choose K_4 as one wishes.

The second observation starts from the identity

$$\begin{aligned}&\mathrm{tr}(\nabla v)^2 + (v.\mathrm{curl}\ v)^2 + |v \times \mathrm{curl}\ v|^2 \\ &\qquad = |\nabla v|^2 + (|v|^2 - 1)|\mathrm{curl}\ v|^2, \end{aligned} \tag{2.6}$$

valid for any suitably smooth $v : \Omega \longrightarrow \mathbb{R}^3$. Hence we can rewrite (1.4) as (here $|u|^2 \doteq 1$ since $u(x) \in S^2$)

$$2\mathcal{W}(u, \nabla u) = (K_1 - K_2 - K_4)(\text{div } u)^2 + K_2|\nabla u|^2 \\ + K_4(\text{tr}(\nabla u)^2) + (K_3 - K_2)|u \cdot \text{curl } u|^2. \quad (2.7)$$

Now if $K_1 = K_2 = K_3$ (the so-called "one constant case"), it is seen that upon choosing $K_4 = 0$

$$2\mathcal{W}(u, \nabla u) = K_2|\nabla u|^2, \quad (2.8)$$

and (1.5) becomes the classical problem of finding minimizing harmonic maps from Ω onto S^2 with prescribed boundary data. We shall return to this problem in the next paragraph.

The identity (2.6) is also useful to show that for $K_4 = \alpha - K_2$, $\alpha = \min(K_1, K_2, K_3)$ and $\beta = 3K_1 + 2K_2 + 2K_3$ we have

$$\alpha|\nabla u|^2 \leqslant 2\mathcal{W}(u, \nabla u) \leqslant \beta|\nabla u|^2. \quad (2.9)$$

Hence for $K_4 = \alpha - K_2$, the energy is coercive in the usual sense. Another important point in the study of (1.5) is the question of ellipticity of the Euler-Lagrange equation associated to this problem. A positive answer is provided in the Appendix of the paper.

Another analytical property of the "one constant case" (see (2.8)) which turns out to be very important in the numerical solution of (1.5) is the following fact:

$$\text{for } K_1 = K_2 = K_3 \text{ and } K_4 = 0, \quad \mathcal{W}\left(\frac{v}{|v|}, \nabla\frac{v}{|v|}\right) \leqslant \mathcal{W}(v, \nabla v) \quad (2.10)$$

for every v such that $|v(x)| \geqslant 1$ for $x \in \Omega$. In general (2.10) does not hold true for arbitrary (K_1, K_2, K_3), but we observe that for our purpose it is sufficient to construct an energy density $\widetilde{\mathcal{W}}$ that satisfies the two properties:

$$\widetilde{\mathcal{W}}(v, \nabla v) = \mathcal{W}(v, \nabla v) \quad \text{when } |v(x)| = 1 \quad \text{for } x \in \Omega, \quad (2.11)$$

and

$$\widetilde{\mathcal{W}}\left(\frac{v}{|v|}, \nabla\frac{v}{|v|}\right) \leqslant \widetilde{\mathcal{W}}(v, \nabla v) \quad (2.12)$$

for every v such that $|v(x)| \geqslant 1$ for $x \in \Omega$. A possible construction follows from the

PROPOSITION 1. – (i) *If* $K_2 \geqslant K_1$ *and* $K_3 \geqslant K_1$, *define*

$$\widetilde{\mathcal{W}}(v, \nabla v) = K_1 \int_\Omega |\nabla v|^2 dx + (K_2 - K_1) \int_\Omega (v.\text{curl } v)^2 dx + (K_3 - K_1) \int_\Omega |v.\nabla v|^2 dx; \tag{2.13}$$

then $\widetilde{\mathcal{W}}$ *satisfies* (2.11)-(2.12) *where* $\mathcal{W}$ *is taken with* $K_4 = K_1 - K_2$.

(ii) *If* $K_1 > K_2$ *or* $K_1 > K_3$, *we set*

$$\widetilde{\mathcal{W}}(v, \nabla v) = K_1 \int_\Omega \left(|v|^2 (\text{div } v)^2 - (\text{div } v) v.\nabla \frac{|v|^2}{2} + \left| \nabla \frac{|v|^2}{2} \right|^2 \right) dx + K_2 \int_\Omega (v.\text{curl } v)^2 dx + K_3 \int_\Omega |v.\nabla v|^2 dx. \tag{2.14}$$

Then $\widetilde{\mathcal{W}}$ *satisfy* (2.11)-(2.12) *where* $\mathcal{W}$ *is taken with* $K_4 = 0$.

REMARK 1. – *In both cases* $\widetilde{\mathcal{W}}(u, F)$ *is a smooth function of* u *and* F, *of the form* (1.2) *and the* $a_{ijkl}(u)$ *are second-degree polynomials in the* u_i. *The proof of Proposition* (1) *is elementary, it relies on the three relations*

$$|v.\nabla v|^2 = |v \times \text{curl } v|^2 \quad if\ |v(x)| = 1, \tag{2.15}$$

$$\left| \frac{v}{|v|} \cdot \nabla \frac{v}{|v|} \right|^2 \leqslant |v.\nabla v|^2 \quad if\ |v(x)| \geqslant 1, \tag{2.16}$$

and

$$\left| \frac{v}{|v|} \cdot \text{curl } \frac{v}{|v|} \right| \leqslant |v.\text{curl } v| \quad if\ |v(x)| \geqslant 1. \tag{2.17}$$

2.2. Review of continuous results

2.2.1. *The general case.* – Following Hardt, Kinderlehrer and Lin [19], [20], it is standard to deduce from (2.9) and the fact that $\mathcal{W}$ is lower semi-continuous on $H^1_\varphi(\Omega; S^2) = \{v \in H^1(\Omega; \mathbb{R}^3), |v(x)| = 1 \text{ a.e. and } v(x) = \varphi(x) \text{ on } \partial\Omega\}$ endowed with its weak topology, that (1.5) admits at least one solution provided $H^1_\varphi(\Omega; S^2)$ is not empty. This will be the case if the function φ is lipschitz on $\partial\Omega$ for example (Lemma 1.1 of [19]).

The next question that arises naturally concerns the smoothness of local and global minimizers. In general these minimizers do not inherit regularity from φ. More precisely, in the case where $\partial\Omega$ is homeomorphic to the sphere S^2, a necessary condition on φ for u to be continuous is that the degree of φ (as a mapping from $\partial\Omega$ into S^2) vanishes. Hence if $\deg(\varphi, \partial\Omega; S^2) \neq 0$, solutions to (1.5) are not continuous in general. From the physical point of view, it can be expected that singularities of u will produce macroscopic phenomena and are therefore of very considerable interest.

Actually the singular set of u cannot be too large and it is shown in [19] that this set is of one dimensional Hausdorff measure zero (and outside of this set the function u is real analytic). Hence lines of singularities are not allowed, and the fact that they can be observed experimentally (see M. Kléman [27]) leads to the following alternative: either one must reconsider the Oseen-Frank model (Ericksen [13] has proposed a new model in this direction which has been studied mathematically by F.-H. Lin [28] and numerically by R. Cohen [7] and K. Godev [16]), or it might happen that the singular set looks like a one dimensional set although it is not (think to a cluster of points).

The hedgehog solution. In the case where Ω is a ball in $\mathbb{R}^3$: $\Omega = \{x \in \mathbb{R}^3, |x-a| < R\}$ a critical point to the energy is known when $\varphi(x) = \frac{x-a}{R}$. The solution (termed as the hedgehog solution) reads

$$u(x) = \frac{x-a}{|x-a|} \tag{2.18}$$

and has a point singularity in the center a of Ω. Let us now describe the results which are known concerning the question whether or not (2.18) solves (1.5). First it follows from Lin [17] that

$$u(x) = \frac{x-a}{|x-a|} \text{ solves (1.5) when } K_1 \leqslant K_2 \text{ and } K_1 \leqslant K_3. \tag{2.19}$$

Second, according to Hélein [24],

$$u(x) = \frac{x-a}{|x-a|} \text{ does not solve (1.5) when } 8(K_1 - K_2) > K_3. \tag{2.20}$$

Finally, Cohen and Taylor [6] (see also Kinderlehrer and Ou [25]) have shown that Hélein's condition is optimal in a certain sense. These properties will be used as tests for our numerical computations.

We have just described how singularities can occur forced by topological obstructions. Surprisingly (at least from the mathematical point of view) singularities can occur even when there are no topological obstructions (see Section 2.2.4). Hence it might be (from the energetical point of view) interesting to develop singularities even when $H^1_\varphi(\Omega; S^2)$ contains smooth (C^∞) functions.

2.2.2. *The "One constant case".* – As already observed, when $K_1 = K_2 = K_3$ the minimization problem (1.5) can be reduced to

$$\operatorname*{Min}_{\substack{u:\overline{\Omega}\to S^2 \\ u=\varphi \text{ on } \partial\Omega}} \int_\Omega |\nabla u|^2 dx. \tag{2.21}$$

In this case the Euler equation associated to (2.19) is simple analytically and reads

$$-\Delta u = u|\nabla u|^2 \quad \text{in } \Omega \tag{2.22}$$

(compare with (A.8) in the Appendix).

Problem (2.21) is the classical problem of finding minimizing harmonic maps from Ω into S^2 with prescribed boundary data. This problem has been studied very extensively from the geometrical point of view (see e.g Eells and Lemaire [12]).

One of the facts we want to point out here is that in general (2.21) has many (possibly infinitely many) solutions. This multiplicity phenomenon must therefore be kept in mind when coming to numerical considerations.

Let us deal now with the question of singularities of solutions. Since we are in a particular case of Section 2.2.1, we expect more precise results, and this will be indeed the case.

2.2.3. *Point singularities.* – A remarkable result of Brezis, Coron and Lieb [5] (see also Schoen and Uhlenbeck [34] when the target manifold is arbitrary) claims that solutions to (2.21) have a finite number of point singularities of hedgehog-type. More precisely for every solution to (2.21), there exist $\varepsilon_j \in \{-1, 1\}, R_j$ rotations in $\mathbb{R}^3$, $a_j \in \Omega$ for $j = 1, ..., N$ and a smooth function v from Ω into $\mathbb{R}^3$ such that

$$u(x) = v(x) + \sum_{j=1}^{N} \varepsilon_j R_j \frac{x - a_j}{|x - a_j|} \tag{2.23}$$

(and $\sum_{j=1}^{N} \varepsilon_j$ is the degree of φ).

This very rigid structure of the solutions to (2.21) follows from the fact that we are dealing with minimizers: Rivière [33] has recently shown that (2.22) admits solutions in $H^1(\Omega; S^2)$ which are discontinuous everywhere in Ω.

2.2.4. *The gap phenomenon.* – As mentioned in Section 2.2.1, the presence of singularities in solutions to (2.21) is not necessarily due to topological obstructions. Indeed Hardt and Lin [22] have constructed a smooth mapping φ on the boundary $\partial\Omega$ of a smooth simply connected domain (a dumb-bell like domain) into the sphere S^2 such that the solutions to (2.21) are singular (hence of the form (2.23) with $\sum_{j=1}^N \varepsilon_j = 0$). It follows that we can expect singular solutions to (2.21) or (1.5) even when the boundary data allows the existence of smooth functions in $H^1_\varphi(\Omega; S^2)$. This phenomenon is termed as "gap phenomenon" since it is related to the possibly strict inequality:

$$\underset{\substack{u:\overline{\Omega}\to S^2 \\ u=\varphi \text{ on } \partial\Omega}}{\text{Min}} \mathcal{E}(u) < \underset{\substack{u \in C^1(\overline{\Omega}; S^2) \\ u=\varphi \text{ on } \partial\Omega}}{\text{Inf}} \mathcal{E}(u). \tag{2.24}$$

Béthuel, Brezis and Coron [4] have introduced a modified energy for which (2.24) is an equality. Quivy [32] has proposed an algorithm which computes critical points of this latter energy and her results support strongly that minimizers of the so-called relaxed energy are smooth functions.

3. A FAMILY OF ALGORITHMS IN THE CONTINUOUS CASE

3.1. Setting of the problem

We would like to solve numerically the Problem (1.5) and in a first step, our purpose is to construct a sequence of mappings: $u^n : \Omega \longrightarrow \mathbb{R}^3$ that satisfy

$$|u^n(x)| = 1 \quad \text{for a.e. } x \in \Omega, \tag{3.1}$$

$$u^n(x) = \varphi(x) \quad \text{for a.e. } x \in \partial\Omega, \tag{3.2}$$

$$\text{the sequence } (u^n) \text{ converges to a solution of } (1.5). \tag{3.3}$$

Such a construction is an algorithm to solve (1.5). We propose below a family of algorithms which will be based on a one step procedure *i.e.* knowing u^n we will be able to find u^{n+1} depending only on u^n (and of course φ and Ω). As it is well known, it is generally hopeless to try to show (3.3) in case of a non convex optimization problem, and the efficiency of the algorithms will be checked by numerical investigations.

3.2. A family of algorithms

Assuming that u^n is known, we are going to look for u^{n+1} as $u^{n+1} = u^n + \delta^n$ where, as it is natural, δ^n is related to the gradient of the energy $\mathcal{E}$ at u^n.

We begin by introducing the following abstract setting. We assume that we are given on $L^2(\Omega)$ a linear self-adjoint unbounded operator A with domain $D(A) = \{v \in L^2(\Omega)\,,\ Av \in L^2(\Omega)\}$ dense in $L^2(\Omega)$. We assume that A is an isomorphism from $D(A)$ (equipped with the graph norm) onto $L^2(\Omega)$ and that A is positive:

$$\int_\Omega (Av)v dx > 0, \quad \forall v \in D(A)\,, \quad v \neq 0.$$

We denote by V the Hilbert space $D(A^{\frac{1}{2}})$ endowed with the norm $|A^{\frac{1}{2}}.|_2$ (we shall denote by $|\,.\,|_p$ the usual norm on $L^p(\Omega)$). Then the dual space V' of V is given by $V' = D\left(A^{-\frac{1}{2}}\right)$ with norm $|A^{-\frac{1}{2}}.|_2$.

• *Example* 1.

We can take $A = -\Delta$ with domain $H^2(\Omega) \cap H_0^1(\Omega)$, where $H_0^1(\Omega) = \{v \in H^1(\Omega)\,,\ v = 0 \text{ on } \partial\Omega\}$. Then $V = H_0^1(\Omega)$, $|A^{\frac{1}{2}}v|_2 = |\nabla v|_2$, and $V' = H^{-1}(\Omega)$.

• *Example* 2.

We can take $A = \Delta^2$ with domain $H^4(\Omega) \cap H_0^2(\Omega)$, where $H_0^2(\Omega) = \{v \in H^2(\Omega) \cap H_0^1(\Omega)\,,\ \nabla v = 0 \text{ on } \partial\Omega\}$. Here $V = H_0^2(\Omega)$, $|A^{\frac{1}{2}}v|_2 = |\Delta v|_2$, $V' = H^{-2}(\Omega)$.

• *Example* 3.

We can take $A = \Delta^2$ with domain $\{v \in H^4(\Omega) \cap H_0^1(\Omega) \text{ and } \Delta v = 0$ on $\partial\Omega\}$. Here $V = H^2(\Omega) \cap H_0^1(\Omega)\,,\ |A^{\frac{1}{2}}v|_2 = |\Delta v|_2$. ■

We refer to the book by J.-L. Lions [31] for details concerning these examples and other classical ones.

We are now able to define the L^2-gradient of the energy $\mathcal{E}$ at a point $v \in H^1(\Omega; S^2)$.

PROPOSITION 2. – *Let v be given in $H^1(\Omega; S^2)$ and assume that*

$$V \subset H_0^1(\Omega) \cap L^\infty(\Omega). \tag{3.4}$$

The limit

$$\langle \text{Grad}_0\, \mathcal{E}(v), w\rangle = \lim_{\varepsilon\to 0} \frac{\mathcal{E}(v+\varepsilon w) - \mathcal{E}(v)}{\varepsilon}, \quad \forall w \in V^3, \tag{3.5}$$

where $\langle\, ,\, \rangle$ *stands for the duality pairing between* V' *and* V, *defines* $\text{Grad}_0\mathcal{E}(v) \in (V')^3$ *and*

$$|\langle \text{Grad}_0\, \mathcal{E}(v), w\rangle| \leqslant K\big(|\nabla v|_2^2\ |w|_\infty + |\nabla v|_2\ |\nabla w|_2\big), \tag{3.6}$$

where the constant K *depends only on* K_1, K_2 *and* K_3 .

Moreover if $K_2 = K_3$ *and* $K_4 = K_3$ *we can replace* (3.4) *by*

$$V \subset H_0^1(\Omega), \tag{3.7}$$

the relation (3.5) *defines again* $\text{Grad}_0\, \mathcal{E}(v) \in V' \subset H^{-1}(\Omega)$, *and*

$$\text{Grad}_0\, \mathcal{E}(v) = -(K_1 - K_3)\nabla(\text{div } v) - K_2\,\Delta v. \tag{3.8}$$

Proof. – For $v \in H^1(\Omega; S^2)$ and $w \in V^3$, the function $\varepsilon \to \mathcal{E}(v+\varepsilon w)$ is a polynomial with respect to ε and we have

$$\begin{aligned} \frac{d}{d\varepsilon}\mathcal{E}(v+\varepsilon w)|_{\varepsilon=0} &= K_1 \int_\Omega (\text{div } v)(\text{div } w)dx \\ &+ 2K_2 \int_\Omega (v.\text{curl } v)(v.\text{curl } w + w.\text{curl } v)dx \\ &+ 2K_3 \int_\Omega (v \times \text{curl } v).(v \times \text{curl } w + w \times \text{curl } v)dx, \end{aligned} \tag{3.9}$$

(note that thanks to (2.2) and since $V \subset H_0^1(\Omega)$, the K_4 term vanishes). The right hand side of (3.9) is then bounded by

$$\begin{aligned} K_1|\text{div } v|_2\ |\text{div } w|_2 &+ 2K_2|\text{ curl } v|_2\ (|\text{curl } w|_2 + |w|_\infty\ |\text{curl } v|_2) \\ &+ 2K_3|\text{curl } v|_2\ (|\text{curl } w|_2 + |w|_\infty\ |\text{curl } v|_2) \end{aligned} \tag{3.10}$$

where we used the fact that $|v|_\infty = 1$. Since we have assumed that $V \subset H_0^1(\Omega) \cap L^\infty(\Omega)$, this estimate shows that $w \to \frac{d}{d\varepsilon}\mathcal{E}(v+\varepsilon w)_{|\varepsilon=0}$ is a linear and continuous form on V^3, *i.e.* an element of $(V')^3$ and we can therefore set (3.5) while (3.6) follows from (3.10).

Concerning now the case where $K_2 = K_3$ and $K_4 = 0$, we make use of the identity (2.6) and find that $\mathcal{E}$ reads in this case as

$$2\mathcal{E}(u) = (K_1 - K_2)\int_\Omega (\text{div } u)^2 + K_2 \int_\Omega |\nabla u|^2 dx. \tag{3.11}$$

Then for $v \in H^1(\Omega; S^2)$ and $w \in V$, we find

$$\frac{d}{d\varepsilon}|_{\varepsilon=0}\, \mathcal{E}(v + \varepsilon w) = (K_1 - K_2)\int_\Omega \text{div } v \text{ div } w\, dx + K_2 \int_\Omega \nabla v.\nabla w\, dx$$

and (3.8) follows readily.

From now on we assume that (3.4) holds true or (3.7) if $K_2 = K_3$ (and then we choose $K_4 = 0$). We take $v \in H_0^1(\Omega; S^2)$ and denote by $K(v)$ the linear closed subspace of V^3:

$$K(v) = \{w \in V^3, w(x).v(x) = 0 \text{ for a.e. } x \in \Omega\} \tag{3.12}$$

i.e. the set of functions in V^3 which are pointwisely orthogonal to v. As explained at the beginning of Section 3.2 we are trying to find how to modify a given u^n in order to decrease the energy. In usual optimization problems, the increment $\delta^n = u^{n+1} - u^n$ is oftenly taken in the opposite direction to the gradient of $\mathcal{E}$ at the point u^n. Here we must ensure that $u^{n+1} \in H_\varphi^1(\Omega; S^2)$ *i.e.* (3.1) and (3.2). Of course (3.2) is a linear constraint which will be satisfied easily by taking $\delta^n = 0$ on $\partial\Omega$ while (3.1) is much more delicate (nonlinear and non-convex). Our method will be to begin by projecting the gradient $\text{Grad}_0\mathcal{E}(u^n)$ on $K(u^n)$ in the following sense. Given $v \in H_\varphi^1(\Omega; S^2)$, we denote by $e(v)$ the solution to the linear programming problem:

Find $e \in V$ such that e solves

$$\min_{w\in K(v)} \left(\frac{1}{2}\langle Aw, w\rangle - \langle \text{Grad}\, \mathcal{E}_0(v), w\rangle\right), \tag{3.13}$$

i.e. the unique element $e(v) \in K(v)$ such that

$$\langle Ae(v) - \text{Grad}\, \mathcal{E}_0(v), w\rangle = 0, \quad \forall w \in K(v), \tag{3.14}$$

where $\langle\, , \rangle$ denotes the duality pairing between V' and V:

$$\langle Af, g\rangle = \int_\Omega (A^{\frac{1}{2}} f).(A^{\frac{1}{2}} g) dx \quad \text{for } f \text{ and } g \text{ in } V.$$

We are now in a position to build our algorithm. We start at some stage with $u^n \in H^1_\varphi(\Omega; S^2)$, set $e_n = e(u^n)$ and take $\tau_n \in \mathbb{R}$ such that

$$\mathcal{E}(u^n - \tau_n e_n) = \min_{t\in\mathbb{R}} \mathcal{E}(u^n - te_n), \tag{3.15}$$

(it is clear that this optimization problem on $\mathbb{R}$ possesses at least one solution). Then we observe that

$$|u^n - \tau_n e_n|(x) = \sqrt{1 + \tau_n^2\, e_n^2(x)} \geqslant 1. \tag{3.16}$$

Hence we can define u^{n+1} by taking

$$u^{n+1}(x) = \frac{u^n(x) - \tau_n e_n(x)}{|u^n(x) - \tau_n e_n(x)|} \quad \text{for a.e. } x \in \Omega. \tag{3.17}$$

Thanks to (3.16) one has

$$|\nabla u^{n+1}|^2(x) \leqslant |\nabla(u^n - \tau_n\, e_n)|^2(x) \quad \text{for a.e. } x \in \Omega \tag{3.18}$$

and then $u^{n+1} \in H^1_\varphi(\Omega; S^2)$. Actually we want also to have $\mathcal{E}(u^{n+1}) \leqslant \mathcal{E}(u^n)$. Obviously, (3.15) gives $\mathcal{E}(u^n - \tau_n e_n) \leqslant \mathcal{E}(u^n)$, but as observed after (2.10), we cannot insure in general that $\mathcal{E}(u^{n+1}) \leqslant \mathcal{E}(u^n - \tau_n e_n)$. Hence we will replace (3.15) by: find t_n such that

$$\widetilde{\mathcal{E}}(u^n - t_n e_n) = \min_{t\in\mathbb{R}} \widetilde{\mathcal{E}}(u^n - te_n) \tag{3.19}$$

where

$$\widetilde{\mathcal{E}}(v) = \int_\Omega \widetilde{\mathcal{W}}(v, \nabla v)dx \tag{3.20}$$

and $\widetilde{\mathcal{W}}$ is given in Proposition 2.1.

Let us summarize the algorithm.

PROPOSITION 3. – *We make one of the hypotheses* (3.4) *or* (3.7) *according to whether $K_2 \neq K_3$ or not. Let u^0 be given in $H^1_\varphi(\Omega; S^2)$, we take $n \geqslant 0$ and assume that $u^n \in H^1_\varphi(\Omega; S^2)$ is known. Let e^n the solution to the minimization problem*

$$\begin{aligned}&\frac{1}{2}\langle Ae^n, e^n\rangle - \langle \mathrm{Grad}_0\mathcal{E}(u^n), e^n\rangle \\ &\quad = \min_{e\in K(u^n)} \frac{1}{2}\langle Ae, e\rangle - \langle \mathrm{Grad}_0\mathcal{E}(u^n), e\rangle. \end{aligned}\tag{3.21}$$

We take t_n *solution to* (3.19) *and set*

$$u^{n+1}(x) = \frac{u^n(x) - t_n e^n(x)}{|u^n(x) - t_n e^n(x)|}. \tag{3.22}$$

Then u^{n+1} *belongs to* $H^1_\varphi(\Omega; S^2)$ *and satisfies*

$$0 \leqslant \mathcal{E}(u^{n+1}) \leqslant \mathcal{E}(u^n) \leqslant \mathcal{E}(u^0). \tag{3.23}$$

The sequence $(u^n)_{n\in\mathbb{N}}$ *is bounded in* $H^1(\Omega; \mathbb{R}^3)$.

REMARK 2. – (i) *Since* (3.21) *can be solved by using* (3.14) *we see that this step reads: find* e^n *such that*

$$\langle Ae^n, w\rangle = \frac{d}{d\varepsilon}\mathcal{E}(u^n + \varepsilon w)|_{\varepsilon=0}, \quad \forall w \in K(u^n) \tag{3.24}$$

and as it is clear in Examples 1, 2 and 3, (3.24) *is a standard variational problem that can be discretized using classical techniques (see Sections 4 and 5).*

(ii) *It might be strange that we use two different energies* $\mathcal{E}$ *and* $\widetilde{\mathcal{E}}$ *in* (3.19) *and* (3.21). *Actually if we take* $\widetilde{\mathcal{E}}$ *instead of* $\mathcal{E}$ *in* (3.21) *we will find the same* e^n. *Indeed, more generally if* $\mathcal{F}$ *and* $\mathcal{E}$ *are two energies which are equal on* $H^1(\Omega; S^2)$ *then*

$$\langle \text{Grad}_0\, \mathcal{F}(v) - \text{Grad}_0 \mathcal{E}(v), w\rangle = 0, \quad \forall w \in K(v). \tag{3.25}$$

This can be checked by writing $\mathcal{F}\left(\frac{v+tw}{|v+tw|}\right) = \mathcal{E}\left(\frac{v+tv}{|v+tw|}\right)$ *for every* $t \in \mathbb{R}$ *and* w *such that* $w.v = 0$ *a.e. in* Ω *and taking the derivative of this equality at* $t = 0$. *Since* $\widetilde{\mathcal{E}}$ *is more involved than* $\mathcal{E}$, *it is more convenient to use* $\mathcal{E}$ *in* (3.24). ■

We have almost given the proof of theorem 3.1 before stating this result. In order to show (3.23) we observe that:

$$\begin{aligned}
&\mathcal{E}(u^{n+1}) = \widetilde{\mathcal{E}}(u^{n+1}) \text{ (by (2.11) since } |u^{n+1}| = 1 \text{ a.e.)},\\
&\widetilde{\mathcal{E}}(u^{n+1}) \leqslant \widetilde{\mathcal{E}}(u^n - \tau_n\, e^n) \text{ (by (2.12) since } |u^n - \tau_n\, e^n| \geqslant 1 \text{ a.e.)},\\
&\widetilde{\mathcal{E}}(u^n - \tau_n\, e^n) \leqslant \widetilde{\mathcal{E}}(u^n) \text{ (by taking } t = 0 \text{ in (3.19))},\\
&\widetilde{\mathcal{E}}(u^n) = \mathcal{E}(u^n) \text{ (again by (2.11))}.
\end{aligned}$$

It follows then from (3.23) and (2.9) that $(u^n)_{n\in\mathbb{N}}$ is bounded in $H^1(\Omega; \mathbb{R}^3)$.

REMARK 3. – *Let us observe that the series* $\sum_{n\geqslant 0}\varepsilon_n$ *is convergent where*

$$0 \leqslant \varepsilon_n = \widetilde{\mathcal{E}}(u^n) - \widetilde{\mathcal{E}}(u^n - \tau_n\, e^n) \tag{3.26}$$

and therefore $\lim_{n\to\infty}\varepsilon_n = 0$.

3.3. Remarks on the convergence (mainly open questions)

Let us first consider the case where $K_1 = K_2 = K_3 = 1$ (the one constant case). If we take the setting of Example 1 (which is allowed since $K_2 = K_3$) we have $\mathrm{Grad}_0\,\mathcal{E}(v) = -\Delta v$, and one sees easily that $t_n = \tau_n = 1$ (see (3.15) and (3.19)). We recover Alouges' algorithms ([1],[2]), and e^n is the solution to

$$\int_\Omega |\nabla(u^n - e^n)|^2 dx = \min_{e\in K(u^n)} \int_\Omega |\nabla(u^n - e)|^2 dx. \tag{3.27}$$

In this case ε_n given in (3.26) is equal to $\frac{1}{2}\int_\Omega |\nabla e^n|^2 dx$ so that

$$\lim_{n\to\infty} e^n = 0 \ \text{ in } H^1(\Omega). \tag{3.28}$$

Since (u^n) is bounded in $H^1(\Omega)$, we can extract a subsequence $(u^{n'})$ which converges to some $u^\infty \in H^1(\Omega)$ in the weak topology of $H^1(\Omega)$ and in the strong topology of $L^2(\Omega)$ and such that $|u^\infty(x)| = 1$ a.e. in Ω. Then one can show that thanks to (3.28), (3.27) implies that the distribution $\sum_{i=1}^3 \frac{\partial}{\partial x_i}\left(\frac{\partial u^{n'}}{\partial x_i} \times u^{n'}\right)$ goes to zero as n' goes to infinity. On the other hand, $\frac{\partial u^{n'}}{\partial x_i} \times u^{n'}$ converges to $\frac{\partial u^\infty}{\partial x_i} \times u^\infty$ in $\mathcal{D}'(\Omega)$; hence $\sum_{i=1}^3 \frac{\partial}{\partial x_i}\left(\frac{\partial u^\infty}{\partial x_i} \times u^\infty\right) = 0$ and since $|u^\infty| = 1$, we conclude that u^∞ is a critical point of $\mathcal{E}$ on $H^1_\varphi(\Omega; S^2)$ whose energy is less than or equal to any of the $\mathcal{E}(u^n)$, $n \in \mathbb{N}$.

REMARK 4. – (i) *Since* $H^1(\Omega; S^2)$ *has no differentiable structure, we must say what do we mean by a critical point of a functional* $\mathcal{F}$ *on* $H^1_\varphi(\Omega; S^2)$. *We say that* v *is a critical point if for every* $\varphi \in \mathcal{D}(\Omega)^3$, *the derivative* $\frac{d}{d\varepsilon}\mathcal{F}(\frac{v+\varepsilon\varphi}{|v+\varepsilon\varphi|})$ *exists at* $\varepsilon = 0$ *and vanishes.*

(ii) *We shall say that the algorithm weakly converges if it is possible to extract a subsequence* $(u^{n'})$ *converging to* $u^\infty \in H^1_\varphi(\Omega; S^2)$ *which is a critical point of* $\mathcal{E}$ *on* $H^1_\varphi(\Omega; S^2)$. ■

Still in the one constant case, we can take one of the setting of Examples 2 or 3 and in both cases $t_n = \tau_n = \frac{\int_\Omega |\Delta e^n|^2 dx}{\int_\Omega |\nabla e^n|^2 dx}$. Moreover ε_n given in (3.26) is equal to $t_n \int_\Omega |\Delta e^n|^2 dx$ and since by a suitable Poincaré inequality there exists a constant $\delta > 0$ which depends only on Ω such that $t_n \geqslant \delta$, we conclude that $\lim_{n\to\infty} e^n = 0$ in $H^2(\Omega)$. We have not been able to prove that this is sufficient (as in the previous case) to conclude that the algorithm is weakly convergent in this setting.

Let us deal now with the case where $K_2 = K_3$. We can again take the setting of Example 1 and we find that e^n solves the variational problem: for every $w \in K(u^n)$,

$$\int_\Omega \nabla e^n.\nabla w dx = K_3 \int_\Omega \nabla u^n.\nabla w dx + (K_1 - K_3) \int_\Omega (\text{div } u^n)(\text{div } w) dx. \tag{3.29}$$

Then, depending on the value of K_1 , we will take either (2.13) or (2.14) in order to construct the energy $\widetilde{\mathcal{E}}$. Since $\widetilde{\mathcal{E}}$ is not quadratic we cannot compute like in the two previous cases t_n (note that $\tau_n = 1$ since $\mathcal{E}$ given in (3.11) is quadratic). Here we have $\varepsilon_n = \widetilde{\mathcal{E}}(u^n) - \widetilde{\mathcal{E}}(u^n - t_n e^n) = t_n(K_3 \int_\Omega |\nabla e^n|^2 dx + (K_1 - K_3) \int_\Omega |\text{div } e^n|^2 dx)$ and assuming that $t_n \geqslant \delta > 0$ independently of n we deduce that $\lim_{n\to\infty} e^n = 0$ in $H^1(\Omega)$. As in the previous case we have not been able to prove that this is then sufficient to conclude that the algorithm is weakly convergent.

Finally we deal with the general case. It is clear that from the numerical point of view, (see the variational problem (3.24)), it will be cheaper to use for A a second order p.d.e. elliptic operator rather than a fourth order one. We were forced in the case where $K_2 \neq K_3$ to take $V \in L^\infty(\Omega) \cap H_0^1(\Omega)$ in order to give a sense to the gradient $\text{Grad}_0\, \mathcal{E}(v)$ for $v \in H^1_\varphi(\Omega; S^2)$. It is clear that if v has better regularity properties we can relax the fact that functions in V are bounded. On the other hand, ∇v cannot be taken much better than square integrable in view of (2.21). More precisely, since the function $\frac{x}{|x|}$ belongs to $W^{1,p}_{\text{loc}}(\mathbb{R}^3)$ for every $p \in [1, 3[$, we cannot expect that a convergent algorithm will support an estimate on $\int_\Omega |\nabla u^n|^3 dx$ (even if $\int_\Omega |\nabla u^0|^3 dx$ is finite).

We start with $u^0 \in W_\varphi^{1,\frac{12}{5}}(\Omega; S^2)$ and observe that the estimate of $\langle \text{Grad}\, \mathcal{E}_0(v), w\rangle$ given by (3.9) can be done as follows (by using Hölder inequality):

$$\begin{aligned}|\langle \text{Grad}_0\, \mathcal{E}(v), w\rangle| &\leqslant K_1 |\text{div } v|_2\, |\text{div } w|_2 \\ &\quad + 2(K_2 + K_3)(|v|^2_\infty\, |\text{curl } v|_2\, |\text{curl} w|_2 + |v|_\infty\, |\text{curl } v|^2_{\frac{12}{5}}\, |w|_6\end{aligned}$$

and since by the Sobolev inequality in 3 dimensions

$$|w|_6 \leqslant C_s(\Omega)|\nabla w|_2, \quad \forall w \in H_0^1(\Omega),$$

we conclude that:

$$|\langle \text{Grad}_0\mathcal{E}(v), w\rangle| \leqslant C_s'(\Omega)(|\nabla v|_2 + |\nabla v|_{\frac{12}{5}})|\nabla w|_2 \tag{3.30}$$

which shows that $\text{Grad}_0\,\mathcal{E}(v) \in H^{-1}(\Omega)$. Hence if $u^0 \in W_\varphi^{1,\frac{12}{5}}(\Omega; S^2)$ we can define $\text{Grad}_0\mathcal{E}(u^0) \in V'$ with $V = H_0^1(\Omega)$ in the setting of Example 1.

At this point, we are able to construct $u^1 = \frac{u^0 - t_0 e^0}{|u^0 - t_0 e^0|}$ as described in Theorem 3.1 and it is worthwhile to observe that (3.18) shows that

$$\int_\Omega |\nabla u^1(x)|^{\frac{12}{5}}\,dx \leqslant \int_\Omega |\nabla(u^0 - t_0 e^0)|^{\frac{12}{5}}\,dx. \tag{3.31}$$

If we assume that e^0 belongs to $W^{1,\frac{12}{5}}(\Omega)$, then $u^1 \in W^{1,\frac{12}{5}}(\Omega)$ and we can iterate the construction.

The hypothesis that we are making is the following: We assume that if $v \in W_\varphi^{1,\frac{12}{5}}(\Omega; S^2)$, the solution $e(v)$ to the variational problem in $K(v)$:

$$\int_\Omega \nabla v.\nabla w\,dx = \frac{d}{d\varepsilon}\mathcal{E}(v + \varepsilon w)|_{\varepsilon=0}, \quad \forall w \in K(v) \tag{3.32}$$

where $K(v) = \{w \in H_0^1(\Omega); w(x).v(x) = 0 \text{ for a.e. } x \in \Omega\}$, belongs to $W^{1,\frac{12}{5}}(\Omega; \mathbb{R}^3)$.

Hence we have the following result:

PROPOSITION 4. – *Under the hypothesis* (3.32), *taking* $u^0 \in W_\varphi^{1,\frac{12}{5}}(\Omega; S^2)$ *and the setting of Example 1, the sequence* (u^n) *constructed via* (3.21), (3.19) *and* (3.22) *satisfies* (3.23) *and is bounded in* $H_\varphi^1(\Omega; S^2)$.

REMARK 5. – *We can remove the hypothesis* (3.32), *replacing the linear problem* (3.14) *by a non-linear one as follows. We take* $p = 9/4$, *and instead of* (3.13), *we solve*

$$\min_{w\in K(v)} \left(\frac{1}{2}||w||_p^2 - \langle Grad_0\mathcal{E}(v), w\rangle\right), \tag{3.33}$$

where $||w||_p^p = \int_\Omega |\nabla w|^p dx$ *(this problem also admits a unique solution). Now starting with* $u^0 \in W_\varphi^{1,p}(\Omega, S^2)$, *we obtain that this time* $\text{Grad}_0\mathcal{E}(u^0) \in W_0^{-1,p'}(\Omega)$, $p' = 9/5$ *and therefore* (3.33) *has a solution* $w^0 \in W_0^{1,p}(\Omega)$. *Next, we solve* (3.19) for $n = 0$ *and set as in* (3.22) $u^1 = \frac{u^0 - \tau_0 w^0}{|u^0 - \tau_0 w^0|}$ *which belongs to* $W_\varphi^{1,9/4}(\Omega, S^2)$.

4. DISCRETE ALGORITHMS AND IMPLEMENTATION

The discretization of the algorithms presented in the last section is mainly straightforward. We work in the finite differences framework (finite elements could be used as well, see Alouges and Coleman [3]). For simplicity the domain Ω is taken to be the three dimensional unit cube $\Omega = [0,1]^3$, and we discretize this domain in equally spaced points:

$$x_{ijk} = (ih, jh, kh)$$

for $0 \leq i \leq M$, $0 \leq j \leq M$, $0 \leq k \leq M$ and $h = \frac{1}{M}$. Then, any vector-field u is discretized by taking its values at the points x_{ijk}

$$u_{ijk} \simeq u(x_{ijk}). \tag{4.2}$$

We approximate the energy $\mathcal{E}_h$ by making the standard order 1 approximation of the derivatives. Namely for all $0 \leq i\,, j\,, k \leq M-1$

$$(\nabla_h u)_{ijk} = \left(\frac{u_{i+1,j,k} - u_{i,j,k}}{h}, \frac{u_{i,j+1,k} - u_{i,j,k}}{h}, \frac{u_{i,j,k+1} - u_{i,j,k}}{h}\right) \tag{4.3}$$

$$\begin{aligned}(\mathrm{curl}_h u)_{ijk} = \Bigg(&\frac{u^3_{i,j+1,k} - u^3_{i,j,k}}{h} - \frac{u^2_{i,j,k+1} - u^2_{i,j,k}}{h},\\ &\frac{u^1_{i,j,k+1} - u^1_{i,j,k}}{h} - \frac{u^3_{i+1,j,k} - u^3_{i,j,k}}{h},\\ &\frac{u^2_{i+1,j,k} - u^2_{i,j,k}}{h} - \frac{u^1_{i,j+1,k} - u^1_{i,j,k}}{h}\Bigg),\end{aligned} \tag{4.4}$$

$$(\mathrm{div}_h u)_{ijk} = \frac{u^1_{i+1,j,k} - u^1_{i,j,k}}{h} + \frac{u^2_{i,j+1,k} - u^2_{i,j,k}}{h} + \frac{u^3_{i,j,k+1} - u^3_{i,j,k}}{h}. \tag{4.5}$$

Here the quantity u^l_{ijk} stands for the l^{th}-component of the vector u_{ijk}.

The energy of configuration (u_{ijk}) is then defined as

$$\begin{aligned}\mathcal{E}_h(u_{ijk}) = \sum_{0\leq i,j,k\leq M-1} &\{K_1(\mathrm{div}_h\ u)^2_{ijk} + K_2(u_{ijk}.(\mathrm{curl}_h u)_{ijk})^2\\ &+ K_3|u_{ijk} \times (\mathrm{curl}_h\ u)_{ijk})|^2\}h^3,\end{aligned} \tag{4.6}$$

and the aim is to minimizing it over the set of all admissible configurations

$$H_h\varphi = \{u_{ijk} \in S^2 \text{such that } u_{ijk} = \varphi_{ijk} \text{ if } x_{ijk} \in \partial\Omega\}. \tag{4.7}$$

For the sake of simplicity, and in order to take advantage of the properties of quadratic functionals, we will from now on use the following expression for $\mathcal{E}_h$:

$$\begin{aligned}\mathcal{E}_h(u_{ijk}) = \sum_{0\le i,j,k\le M-1} &\{K_1(\text{div}_h\ u)^2_{ijk}\\ &+ (K_2 - K_3)(u_{ijk}.(\text{curl}_h\ u)_{ijk})^2\\ &+ K_3|(\text{curl}_h\ u)_{ijk}|^2\}h^3.\end{aligned} \tag{4.8}$$

All this setting is very standard and has been extensively used by several authors in the field [1][2][8][9][10][32][30].

In the one constant case, we simply use the energy.

$$\mathcal{E}_h\,(u_{ijk}) = \sum_{0\le i,j,k\le M-1} |(\nabla_h u)_{ijk}|^2 h^3. \tag{4.9}$$

Moreover the space where the increment is computed writes for a given configuration v_{ijk} as

$$K_h(v_{ijk}) = \{w_{ijk}, w_{ijk}.v_{ijk} = 0, w_{ijk} = 0 \text{ if } x_{ijk} \in \partial\Omega\}. \tag{4.10}$$

Eventually, in order to be able to write the discrete version of the algorithm presented above in a continuous framework, we need on $H_{h\varphi}$ a positive-definite operator A_h.

We are now in a position to write the algorithm

- Start with an initial configuration u^0_{ijk}.
- Solve the following problem:

$$\min_{w_{ijk}\in K_h(v_{ijk})} \frac{1}{2}\big(\langle A_h\, w_{ijk}, w_{ijk}\rangle_h - \langle \text{Grad } \mathcal{E}_h(u^n_{ijk}), w_{ijk}\rangle_h\big) \tag{4.11}$$

and call w^n_{ijk} the solution.

- Compute $u^{n+1}_{ijk} = \frac{u^n_{ijk} - t_n\, w^n_{ijk}}{|u^n_{ijk} - t_n w^n_{ijk}|}$

where t_n has been obtained in order to minimize $\mathcal{E}_h(u^n_{ijk} - tw^n_{ijk})$, $t \in \mathbb{R}$. In this algorithm the notation $\langle \, , \, \rangle_h$ stands for any inner product on $H_{h\varphi}$, and Grad $\mathcal{E}_h(u^n_{ijk})$ means the quantity such that

$$\langle \mathrm{Grad}\, \mathcal{E}_h(u_{ijk}), w_{ijk} \rangle_h = \lim_{t \longrightarrow 0} \frac{\mathcal{E}_h(u_{ijk} + tw_{ijk}) - \mathcal{E}_h(u_{ijk})}{t} \tag{4.12}$$

REMARK 6. – (i) *The algorithm presented above may be viewed as a projected preconditioned gradient algorithm. Indeed the operator A_h plays the role of a preconditioner. This was not the case in the previous Section where the operator A was necessary to be able to give a meaning to the algorithms.*

(ii) *We could take an operator changing at each iteration A^n_h instead of A_h. We would have obtained what is called a variable metric algorithm in the literature. However, in most of the following computations, taking $A_h = -\Delta_h$ (the discrete Laplace operator turns out to be sufficient).*

(iii) *It could seem strange to minimize on $t \in \mathbb{R}$, $\mathcal{E}_h\,(u^n_h - tw^n_h)$ and then project (instead of minimizing $\mathcal{E}_n(\frac{u^n_h - tw^n_h}{|u^n_h - tw^n_h|})$). The advantage of the former problem is that explicit formulas can be given to compute the optimal value of t in the case of quadratic energies (when $K_2 = K_3$). Moreover, even in the general case it is slightly of less cost than the latter problem. At last, the numerical experiments we made to compare both formulations did not give preference to one upon the other (in terms of rate of convergence of the algorithms).*

(iv) *In the special quadratic case of* (4.9), *we can compute for a given operator A_h the explicit value of t_n (when minimizing the energy along the direction w^n_h). In [2], we give results in the case where $A_h = -\Delta_h$ is the classical 7-point discrete Laplace operator. The linear operator being the gradient of the energy, we easily get the optimal value of t_n*

$$t_n = 1. \tag{4.13}$$

This of course saves a lot of computations and speeds up the algorithm.

5. NUMERICAL RESULTS

5.1. Resolution of Problem (4.11)

We recall the problem (4.11) which contains most of the computational cost

$$\min_{w_h \in K_h(u_h)} \frac{1}{2}(\langle A_h w_h, w_h \rangle_h - \langle \mathrm{Grad}\mathcal{E}_h(u_h), w_h \rangle_h), \tag{5.1}$$

where u_h is an admissible configuration.

As explained previously, the solution w_h is also the unique element in $K_h(u_h)$ such that

$$\langle A_h w_h - \text{Grad } \mathcal{E}_h(u_h), v_h\rangle_h = 0, \quad \forall v_h \in K_h(u_h), \tag{5.2}$$

or equivalently

$$P_h(u_h)A_h w_h = P_h(u_h)\text{Grad}\mathcal{E}_h(u_h), \quad w_h \in K_h(u_h), \tag{5.3}$$

where $P_h(u_h)$ is the pointwise projection onto the plane orthogonal to u_h. Equation (5.13) is a linear equation (the operator $P_h(u_h)A_h$ is linear) and the constraint $w_h \in K_h(u_h)$ is also linear (we can write it as $P_h(u_h)w_h = 0$). As we did in [2], we write a conjugate gradient algorithm in order to solve this problem. Notice that the configuration u_h is given:

- Start with an initial guess w_h^0
- Compute $r_h^0 = P_h(\text{Grad}\,\mathcal{E}(u_h) - A_h\, w_h^0)$, $p_h^0 = r_h^0$
- Set for all $n \geq 0$

$$\left.\begin{aligned} \alpha^n &= \frac{\| r_h^n \|_h^2}{\langle P_h(u_h)A_h p_h^n, p_h^n\rangle_h}, \\ w_h^{n+1} &= w_h^n + \alpha^n p_h^n, \\ r_h^{n+1} &= r_h^n - \alpha^n P_h(u_h)A_h p_h^n, \\ p_h^{n+1} &= r_h^{n+1} + \frac{\|r_h^{n+1}\|_h^2}{\|r_h^n\|_h^2} p_h^n. \end{aligned}\right\} \tag{5.4}$$

Here, $\| \,.\, \|_h$ denotes the norm associated to the inner product $\langle .,. \rangle_h$

$$\| r_h \|_h^2 = \langle r_h, r_h\rangle_h. \tag{5.5}$$

The following picture shows a typical rate of convergence of this conjugate gradient routine to solve one of the problem (P_h) arising in our applications (we have taken $A_h = -\Delta_h$). In our computations, this stage doesn't seem to be of prohibitive cost compared to the line-search routine.

5.2. Representation of the vector fields

As done in [1] and [2], the solutions are drawn by plotting in the unit cube few of its fibers. One of the main advantages of drawing fibers of the maps is that it allows a direct view of the singularities of the solution, at least when this solution is not too chaotic (The mathematical properties of the fibers has also been studied by Gulliver [17], [18]).

DEFINITION 1. – *Let* $u \in H^1_\varphi(\Omega, S^2)$, *we call*

$$F_u(s) = u^{-1}(\{s, -s\})$$

the fiber of u *associated to a vector* $s \in S^2$.

Generically, since Ω is of dimension 3, these fibers are curves in Ω.

A classical example: if we consider the map

$$\begin{aligned} u_* : \Omega &\longrightarrow S^2 \\ x &\longrightarrow \frac{x}{|x|}, \end{aligned}$$

the fibers of u_* are obviously straight lines that are crossing each other at 0. As discussed in [2], this is quite general since if two fibers cross each other at a point, then the map has to take several values at this point. In other words, the map has a singularity. Conversely, if x is a singularity of degree k of a map u, then on any sufficiently small ball around x, u maps k times the sphere S^2. This means that any fiber crosses k times at x.

5.3. Symmetry breaking

As described in Section 2.2.1, the hedgehog map ($u_* : x \to \frac{x}{|x|}$) is always (with respect to the K_i) a critical point of the energy. However, this symmetric solution loses its local minimizing property when $8(K_2 - K_1) + K_3$ becomes negative. Our algorithms will be tested upon this fact. We observe that only the local minimizing property has been studied from the analytical point of view while nothing is known on the global minimizing property (beside the very particular case where $K_1 = K_2 = K_3$). In every calculation shown hereafter, the starting configuration has been taken to be u_* whose three fibers are shown in Figure 2. Then, we took few sets of constants K_i and run the algorithm.

5.3.1. *Preponderant or negligible splay.* – We study the case where K_2 and K_3 are of the same order of magnitude whereas K_1 is different. Hence splay costs more or less energy. Two sets of constants have been taken in this case, $K_i = (10, 1, 1)$ and $K_i = (1, 10, 10)$. We show in both cases the fibers of the final map in Figures 3 and 4.

Not surprisingly, in the former case u_* is not minimizing whereas it seems to be minimizing in the latter case. This is in perfect accordance with Hélein's condition (2.20).

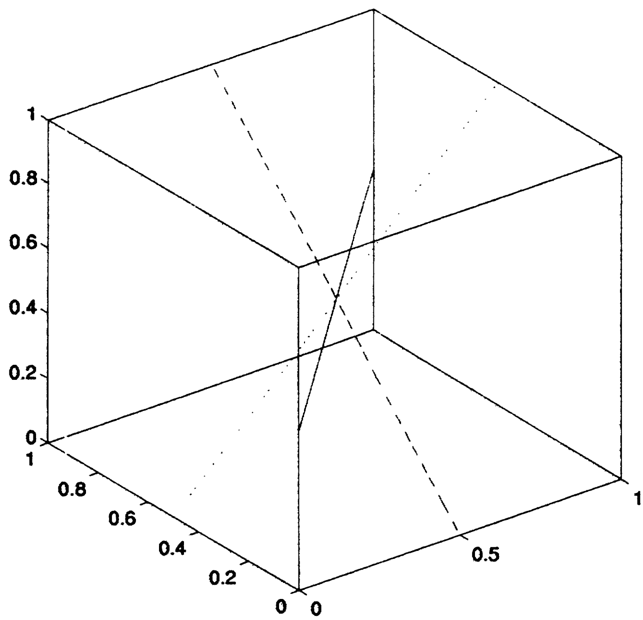

Fig. 2. – u_* is the initial configuration.

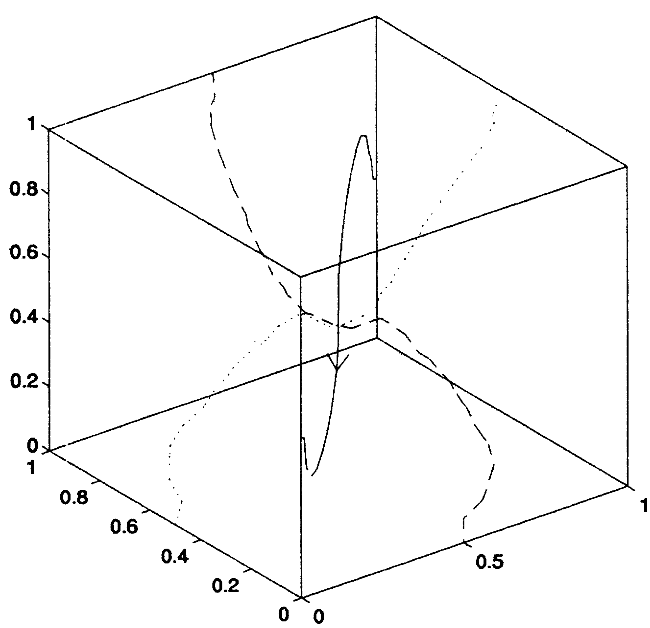

Fig. 3. – Final configuration for $K_1 = 10$, $K_2 = 1$ and $K_3 = 1$.

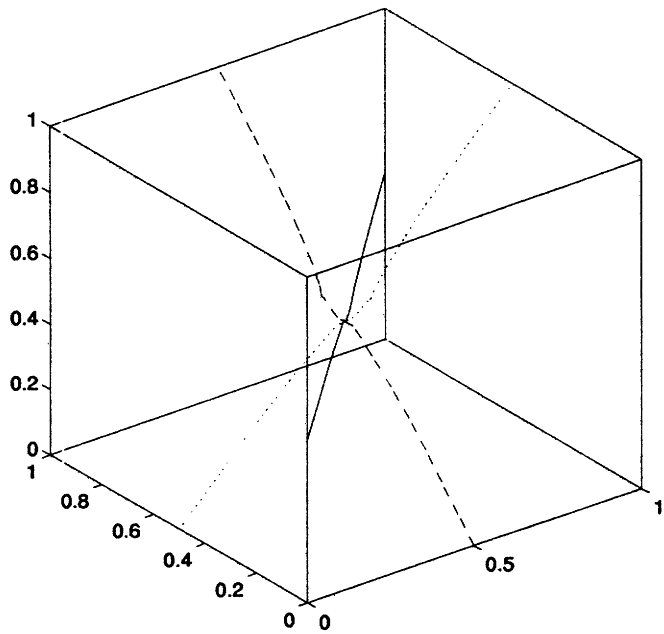

Fig. 4. – Final configuration for $K_1 = 1$, $K_2 = 10$ and $K_3 = 10$.

5.3.2. *Preponderant or negligible bend.* - Let us investigate the case where K_1 and K_3 are of the same order of magnitude and K_2 is different. This situation allows or forbids bending to occur. The final maps obtained by the algorithm are shown for the two sets of constants $K_i = (1, 10, 1)$ and $K_i = (10, 1, 10)$ respectively in Figures 5 and 6. The results are still in accordance with Hélein's condition since u_* seems to be minimizing in the first case and bending occurs in the second.

5.3.3. *Preponderant or negligible twist* – This section corresponds to the situation where K_1 and K_2 are of the same order of magnitude and K_3 is different. As before we experimented two sets of constants $K_i = (1, 1, 10)$ and $K_i = (10, 10, 1)$. The results are presented in Figure 7 for the first set of constants, and in Figure 8 for the second. In this latter case, it is seen that the algorithm succeeds in decreasing sensibly the energy (of an amount of about 10%) for a set of constants that does not violate Hélein's condition. This seems to indicate that the initial map is not the global minimizer even if it is a local minimizer in the sense given in [6]. Numerically speaking the relation (2.20) does not seem to be optimal. Furthermore, the final map shows a complicated behavior that "looks like" a line singularity.

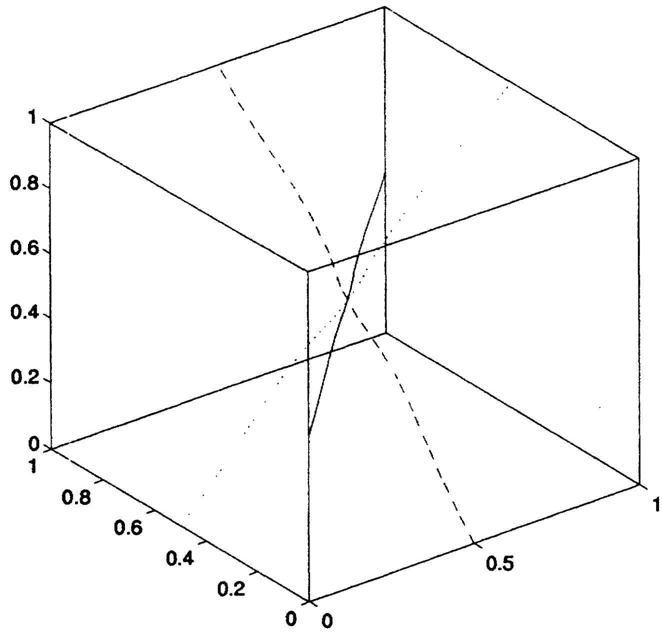

Fig. 5. – Final configuration for $K_1 = 1$, $K_2 = 10$ and $K_3 = 1$.

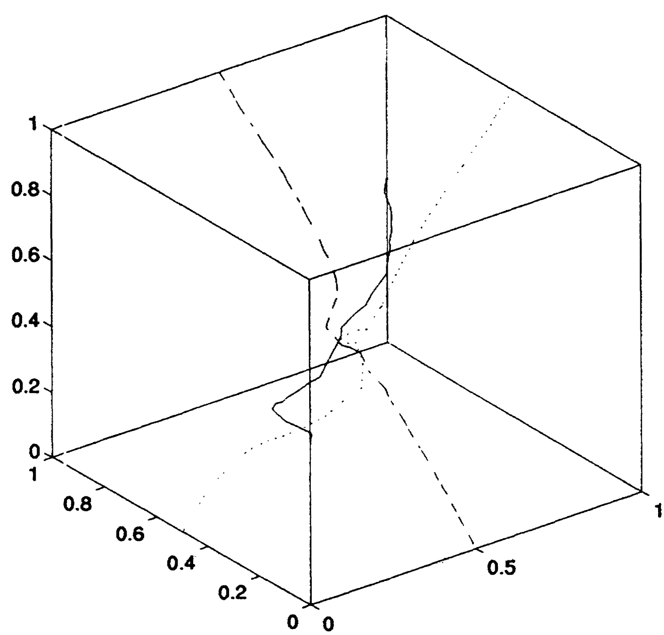

Fig. 6. – Final configuration for $K_1 = 10$, $K_2 = 1$ and $K_3 = 10$.

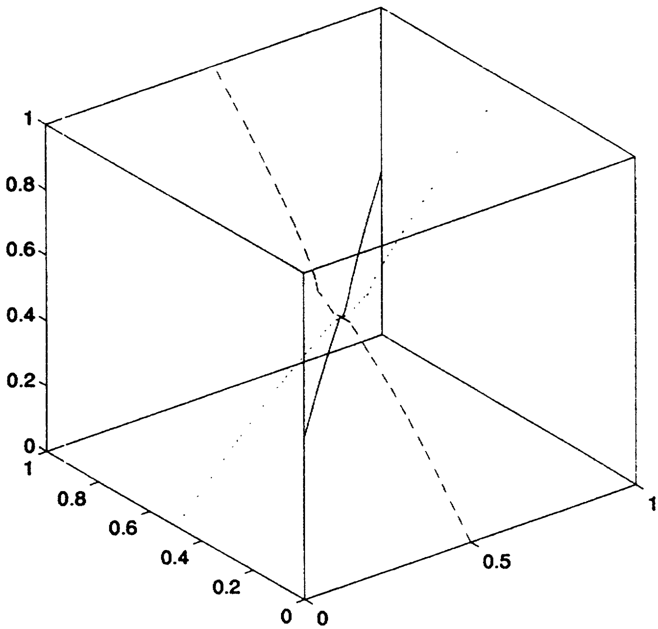

Fig. 7. – Final configuration for $K_1 = 1$, $K_2 = 1$ and $K_3 = 10$.

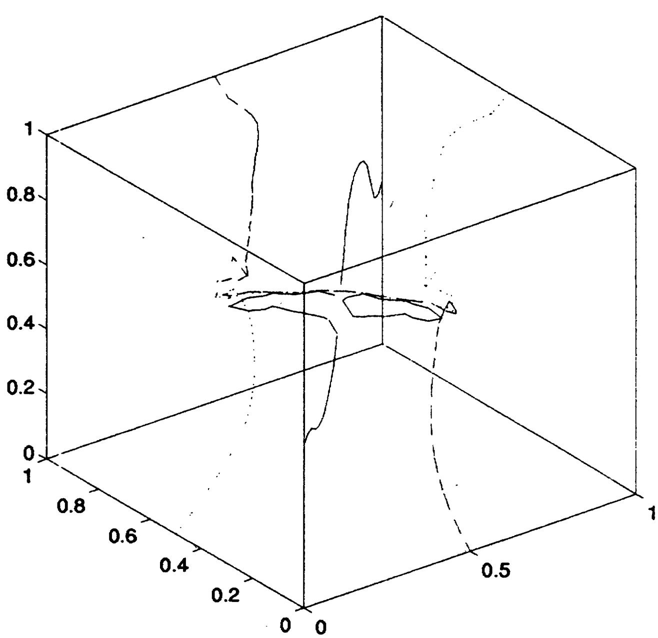

Fig. 8. – Final configuration for $K_1 = 10$, $K_2 = 10$ and $K_3 = 1$.

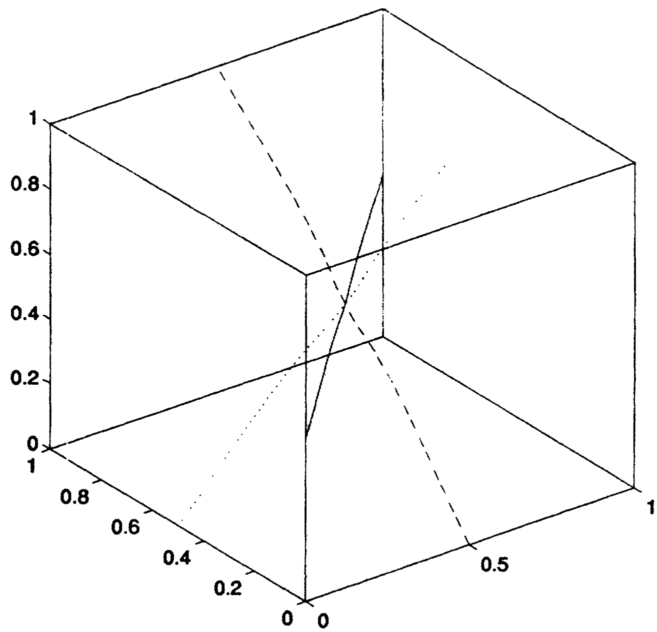

Fig. 9. – Final configuration for PAA 120°C.

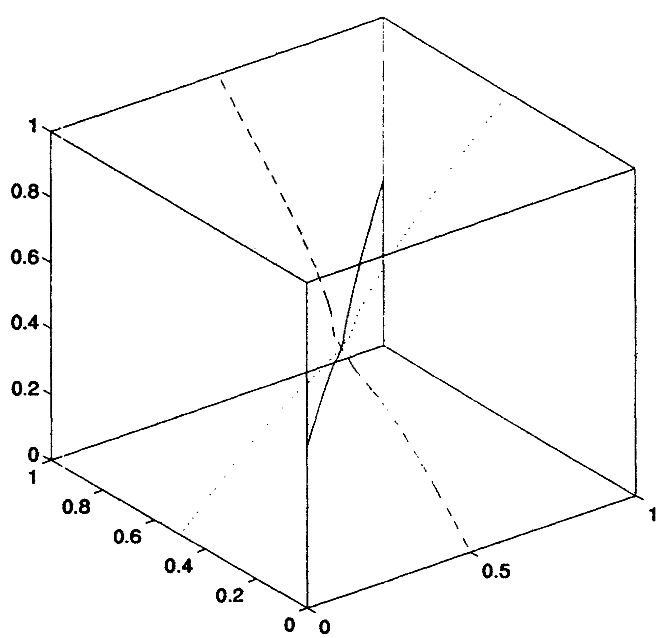

Fig. 10. – Final configuration for PAA 125°C.

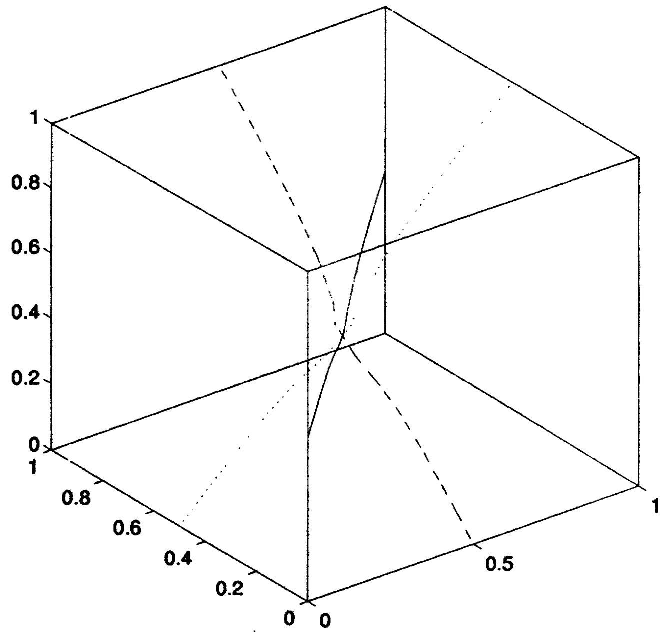

Fig. 11. – Final configuration for PAA 129°C.

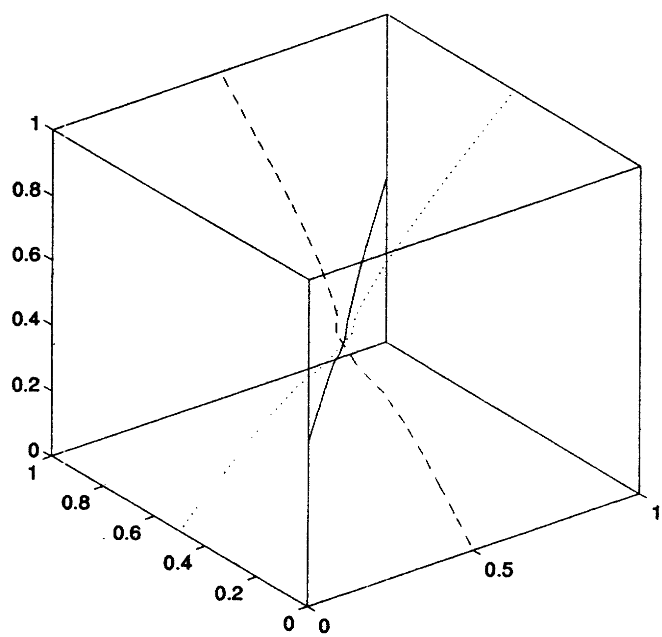

Fig. 12. – Final configuration for MBBA 22°C.

TABLE 2

Decay of the energy for the different values of constants.

K_1	K_2	K_3	E_{ini}	E_{fin}	$\text{sign}(8(K_2 - K_1) + K_3)$
10	1	1	147.479	127.170	−
1	10	10	15.573	15.281	+
1	10	1	14.857	14.805	+
10	1	10	148.380	140.210	−
1	1	10	15.556	15.273	+
10	10	1	147.515	134.767	+
5	3.8	10.1	74.647	74.519	+
4.5	2.9	9.5	67.215	66.103	−
3.85	2.4	7.7	57.470	56.530	−
5.3	2.2	7.45	78.841	77.614	−

5.3.4. *Concerning p-azoxyanisole (PAA) and N-(p-methoxybenzylindene)-p-butylaniline (MBBA).* – We end this section by showing the results obtained using the values of the constants given in Table 1. As the algorithm is independant of the normalization of the constants, we multiply all of them by 10^7 in order to have them of order one. The four cases are respectively given in Figures 9, 10, 11 and 12. As expected from the values of the constants, for the PAA, a symmetry breaking occurs when the temperature increases. Although this is not very obvious from the pictures, the decay of energy is significative in the cases where Hélein's condition is not satisfied. The Table 2 eventually summarizes the decay of the energy for all the test cases presented here.

6. OPEN QUESTIONS AND FUTURE INVESTIGATIONS

As pointed out just above, Hélein's condition seems to be not optimal from the computational point of view. We think that such a question should be investigated analytically.

In Section 3.3, we have given a set of questions related to the convergence of the algorithms. We believe that these problems are connected with deep questions concerning possible compensations in the related Euler equations, whose theory has not yet been addressed.

A natural continuation of this work is to study the influence of either a magnetic or an electric field (or even both) on the stable configurations.

Similar questions (the unknown is also a unit vector) occur in micro-magnetism. Such problems are currently under investigation.

APPENDIX

Ellipticity of the Euler equation

Our aim in this Appendix is to show that the Euler equation associated with the Problem (1.5) is indeed elliptic. The key observation is that if u solves (1.5) for a certain value of K_4, it solves (1.5) for every value of K_4 (see the beginning of Section 2.1). In order to emphasize this fact we denote here

$$\mathcal{E}_\alpha(u) = \int_\Omega \mathcal{W}_\alpha(u, \nabla u)\, dx, \tag{A.1}$$

where

$$\mathcal{W}_\alpha(u, \nabla u) = \frac{1}{2}\alpha|\nabla u|^2 + \mathcal{V}_\alpha(u, \nabla u), \tag{A.2}$$

and

$$\begin{aligned} 2\,\mathcal{V}_\alpha\,(u, \nabla u) =& (K_1 - \alpha)(\text{div}u)^2 + (K_2 - \alpha)(u.\text{curl}u)^2 \\ &+ (K_3 - \alpha)|u \times \text{curl}u|^2 \\ &+ (K_2 + K_4 - \alpha)(\text{tr}(\nabla u)^2 - (\text{div}u)^2). \end{aligned} \tag{A.3}$$

Hence the problems (where α varies)

$$\min_{u \in H^1_\varphi(\Omega; S^2)} \mathcal{E}_\alpha(u) \tag{A.4}$$

have the *same solutions.*

In order to obtain an Euler equation associated with (A.4), we need to make some infinitesimal perturbations on solutions to this problem. Unfortunately $H^1_\varphi\,(\Omega; S^2)$ has no differentiable structure and therefore we use the fact that for every $\varphi \in H^1_0\,(\Omega; \mathbb{R}^3) \cap L^\infty(\Omega; \mathbb{R}^3)$, if u solves (1.5), then the derivative of the function

$$\varepsilon \longrightarrow \mathcal{E}_\alpha\left(\frac{u + \varepsilon\,\varphi}{|u + \varepsilon\,\varphi|}\right)$$

(which is defined for $|\varepsilon|$ small) must vanish at $\varepsilon = 0$. We then obtain that a solution u of (A.3) satisfies: for every $\varphi \in H_0^1(\Omega; \mathbb{R}^3) \cap L^\infty(\Omega; \mathbb{R}^3)$,

$$\int_\Omega [D_2 \mathcal{W}_\alpha(u, \nabla u).\nabla\varphi + D_1 \mathcal{W}_\alpha(u, \nabla u).\varphi - \lambda u.\varphi] dx = 0, \qquad \text{(A.5)}$$

where λ is a scalar function on Ω that we will explicit below. Let us take in particular $\varphi = \eta u$ where $\eta \in \mathcal{D}(\Omega)$, we obtain

$$\int_\Omega \{(D_2 \mathcal{W}_\alpha(u, \nabla u).\nabla u + D_1 \mathcal{W}_\alpha(u, \nabla u).u - \lambda)\eta + D_2 \mathcal{W}_\alpha(u, \delta u).(u \otimes \nabla\eta)\} dx = 0 \qquad \text{(A.6)}$$

Using the fact that $|u(x)|^2 = 1$ for $a.e.\, x \in \Omega$, we find that

$$\lambda = -\mathrm{div}(u\, D_2 \mathcal{V}_\alpha(u, \nabla u)) + D_2 \mathcal{W}_\alpha(u, \nabla u).\nabla u + D_1 \mathcal{W}_\alpha(u, \nabla u).u. \qquad \text{(A.7)}$$

Returning to (A.5), we deduce the Euler-Lagrange equation associated with (A.4):

$$\begin{aligned} &- \mathrm{div}[D_2 \mathcal{W}_\alpha(u, \nabla u) - (u\, D_2 \mathcal{V}_\alpha(u, \nabla u)) \otimes u] + D_1 \mathcal{W}_\alpha(u, \nabla u) \\ &= [D_2 \mathcal{W}_\alpha(u, \nabla u).\nabla u + D_1 \mathcal{W}_\alpha(u, \nabla u).u]u \\ &\quad + \nabla u.(u\, D_2 \mathcal{V}_\alpha(u, \nabla u)). \end{aligned} \qquad \text{(A.8)}$$

This system of equations is a particular case of systems of the type

$$\frac{\partial}{\partial x_i}\left(a_{ij}^{kl}(u)\frac{\partial u_k}{\partial xj}\right) + b_l(u, \nabla u) = 0, \quad \text{for } l = 1, 2, 3. \qquad \text{(A.9)}$$

At this point we recall the classical definition of elliptic systems (see e.g. Giaquinta [15], [23]).

DEFINITION A.1. – *The system* (A.9) *is said to be strongly elliptic if there exists* $\gamma > 0$ *such that for a.e.* $x \in \Omega$,

$$\sum_{i,j,k,l=1}^{3} a_{ij}^{kl}(u(x))\xi_i\, \xi_j\, \eta_k \eta_l \geq \gamma, \quad \forall\, \xi, \eta \in S^2,$$

in such a case γ *is a constant of strong ellipticity of* (A.8).

We can now state the following result (compare with Hardt-Kinderlehrer [23]):

THEOREM A.1. – *For* $\alpha = \frac{K_1+K_3}{2}$, *the Euler-Lagrange equation* (A.7) *is strongly elliptic with constant of ellipticity* γ *equal to Min* (K_1, K_2, K_3).

In order to show this theorem, we observe that it is only the divergence term in (A.7) which is important.

Hence the proof will follow from the identity:

$$(D_2\mathcal{W}_\alpha(u,\xi\otimes\eta) - uD_2\mathcal{V}_\alpha(u,\xi\otimes\eta)\otimes u).\xi\otimes\eta \geq \gamma \qquad \text{(A.10)}$$

for $u : \Omega \longrightarrow S^2$ and ξ, η arbitrary on S^2. This condition can be explicited as

$$\alpha + (D_2\,\mathcal{V}_\alpha(u,\xi\otimes\eta) - uD_2\,\mathcal{V}_\alpha(u,\xi\otimes\eta)\otimes u)).\xi\otimes\eta \geq \gamma \qquad \text{(A.11)}$$

for $\xi, \eta \in S^2$.

In order to show (A.11), we split $\mathcal{V}_\alpha$ into four parts:

$$\mathcal{V}_\alpha\,(u,p) = \mathcal{V}_{1\alpha}(u,p) + \mathcal{V}_{2\alpha}(u,p) + \mathcal{V}_{3\alpha}(u,p) + \mathcal{V}_{4\alpha}\,(u,p)$$

with

$$\mathcal{V}_{1\alpha}\,(u,p) = \frac{1}{2}\beta_1\,(\mathrm{tr}(p))^2, \qquad \text{(A.12)}$$

$$\mathcal{V}_{2\alpha}\,(u,p) = \frac{1}{2}\beta_2\,(u.\Lambda(p))^2,$$

$$\mathcal{V}_{3\alpha}\,(u,p) = \frac{1}{2}\beta_3\,|u\times\Lambda(p)|^2, \qquad \text{(A.13)}$$

and

$$\mathcal{V}_{4\alpha}(u,p) = \frac{1}{2}\,\beta_4(\mathrm{tr}(p^2) - (\mathrm{tr}(p))^2).$$

Here the coefficients β_i are simply

$$\beta_1 = K_1 - \alpha, \quad \beta_2 = K_2 - \alpha, \quad \beta_3 = K_3 - \alpha, \quad \beta_4 = K_2 + K_4 - \alpha,$$

tr is the trace operator on 3×3 matrices, and Λ is defined on 3×3 matrices by

$$\Lambda(p) = \begin{pmatrix} p_{23} - p_{32} \\ p_{31} - p_{13} \\ p_{12} - p_{21} \end{pmatrix}.$$

Using the relation

$$(u\, D_2\, \mathcal{V}_{i\alpha}(u, \xi \otimes \eta) \otimes u).\xi \otimes \eta = (\xi.u) D_2\, \mathcal{V}_{i\alpha}(u, \xi \otimes \eta).u \otimes \eta$$

for all $1 \leq i \leq 4$, we get

$$\begin{aligned}(D_2 \mathcal{V}_{1\alpha}(u, \xi \otimes \eta) - u D_2 \mathcal{V}_{1\alpha}(u, \xi \otimes \eta) \otimes u).\xi \otimes \eta \\ = \beta_1((\xi.\eta)^2 - (\xi.\eta)(\xi.u)(u.\eta)).\end{aligned}$$

The second term is in the same way

$$\begin{aligned}(D_2 \mathcal{V}_{2\alpha}(u, \xi \otimes \eta) - u D_2 \mathcal{V}_{2\alpha}(u, \xi \otimes \eta) \otimes u).\xi \otimes \eta \\ = \beta_2((u.(\xi \times \eta))^2 - (\xi.u)((u.(\xi \times \eta))(u.(u \times \eta)) \\ = \beta_2(u.(\xi \times y))^2.\end{aligned} \tag{A.14}$$

The third term gives the following contribution:

$$\begin{aligned}(D_2 \mathcal{V}_{3\alpha}(u, \xi \otimes \eta) - u D_2 \mathcal{V}_{3\alpha}(u, \xi \otimes \eta) \otimes u).\xi \otimes \eta \\ = \beta_3(|u \times (\xi \otimes \eta)|^2 - (\xi.u)(u \times (\xi \times \eta)).(u \times (u \times \eta))) \\ = \beta_3((u.\eta)^2 - (u.\eta)(u.\xi)(\xi.\eta))\end{aligned}$$

The fourth term gives no contribution, since

$$\begin{aligned}D_2 \mathcal{V}_{4\alpha}(u, \xi \otimes \eta).\xi \otimes \eta = \beta_4(\mathrm{tr}((\xi \otimes \eta)^2) - (\mathrm{tr}(\xi \otimes \eta))^2) \\ = \beta_4((\xi.\eta)^2 - (\xi.\eta)^2) = 0\end{aligned}$$

and

$$D_2 \mathcal{V}_{4\alpha}(u, \xi \otimes \eta).u \otimes \eta = \beta_4((\eta.u)(\xi.\eta) - (\xi.\eta)(u.\eta)) = 0.$$

Thus, we are led to prove that there exists a positive constant γ such that for any $(u, \eta, \xi) \in (S^2)^3$

$$I(\xi, \eta, u) = \alpha + \beta_1((\xi.\eta)^2 - (\xi.u)(u.\eta)(\xi.\eta)) + \beta_2(u.(\xi \otimes \eta))^2 \quad (A.15)$$
$$+\beta_3((u.\eta)^2 - (u.\eta)(u.\xi)(\xi.\eta)) \quad (A.16)$$

satisfies

$$I(\xi, \eta, u) \geq \gamma. \quad (A.17)$$

The key point now is that we can choose any value for α. Hence taking $\alpha = \frac{K_1+K_3}{2}$, we obtain replacing this value in (A.15)

$$I(\xi, \eta, u) = \frac{K_1 + K_3}{2} + \frac{K_1 - K_3}{2}((\xi.\eta)^2 - (u.\eta)^2)$$
$$+ \left(K_2 - \frac{K_1 + K_3}{2}\right) \det(\xi, \eta, u)^2.$$

We then have two possibilities:

First

$$\beta_2 = K_2 - \frac{K_1 + K_3}{2} \geq 0, \quad (A.18)$$

then

$$I(\xi, \eta, u) \geq \frac{K_1 + K_3}{2} - \frac{|K_1 - K_3|}{2} = \text{Min}(K_1, K_3) \quad (A.19)$$
$$= \text{Min}(K_1, K_2, K_3). \quad (A.20)$$

Second

$$\beta_2 = K_2 - \frac{K_1 + K_3}{2} \leq 0, \quad (A.21)$$

then we suppose $K_1 \geq K_3$ and work with u and η (if $K_1 \leq K_3$ we work with ξ and η). Let us call θ the angle between u and η, we have

$$I(\xi, \eta, u) \geq \frac{K_1 + K_3}{2} - \frac{K_1 - K_3}{2} \cos^2 \theta + \left(K_2 - \frac{K_1 + K_3}{2}\right) \sin^2 \theta$$
$$= K_3 \cos^2 \theta + K_2 \sin^2 \theta \geq \text{Min}(K_2, K_3) = \text{Min}(K_1, K_2, K_3)$$

The case $K_1 \leq K_3$ works in the same way.

Theorem (A.1) is proved.

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