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MATHEMATICAL PROBLEMS OF LIQUID CRYSTALS

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0. INTRODUCTION. Today, everyone is familiar with the display devices (calculators, watches, etc.) using liquid crystals. Such materials are composed of rod-like molecules. These molecules enjoy an orientational order -unlike usual liquids- but they do not have the strict configurational order of solids. The orientation of the molecules (more precisely their optic axes) is well defined and varies smoothly except at isolated points (or possibly lines) called the "defects" which are easily identified in experiments. We represent the orientation of the molecule sitting at $x \in \Omega$ (Ω is the region occupied by the liquid crystal) by a point $u(x)$ of S^2, the unit sphere of $\mathbb{R}^3$. Strictly speaking, one should use a point of the projective plane $\mathbb{R}P^2$ since $u(x)$ and $-u(x)$ are physically indistinguishible, but we shall ignore this difficulty.

Every configuration has a "deformation energy" :

$$E_{OF}(u) = \int_\Omega W(u(x), \nabla u(x))dx \tag{1}$$

where W, the Oseen-Frank bulk energy density, is given by

$$W(u, \nabla u) = K_1(div\, u)^2 + K_2(u \cdot curl\, u)^2 + K_3|u \times curl\, u|^2 + \alpha[tr(\nabla u)^2 - (div\, u)^2].$$

Here K_1, K_2, K_3 and α are positive constants depending on the material. In fact, W is the most general expression which is quadratic in ∇u (with coefficients depending on u) and invariant under the canonical transformations. In addition one prescribes a boundary condition, usually the Dirichlet condition, $u = g$ on $\partial\Omega$, which is physically realistic.

It is reasonable to assume that equilibrium configurations correspond to critical points of the energy, i.e. $\delta E_{OF}(u) = 0$, and that the stable ones correspond to minimizes of the energy ; see however the discussion in Section 4.

For a detailed presentation of the physics we refer to the books by Chandrasekhar [14], De Gennes [17] and Kleman[32], to the articles in the special volume edited by Ericksen-Kinderlehrer [23] and to the papers [13], [21], [22], [31].

In the special case where $K_1 = K_2 = K_3 = \alpha = 1$ (the one constant approximation) the energy becomes

$$E(u) = \int_\Omega |\nabla u|^2 \, dx \tag{2}$$

and its Euler equation $\delta E = 0$ under the constraint $u(x) \in S^2$ is

$$-\Delta u = u|\nabla u|^2$$

i.e. the equation of *harmonic maps* from Ω to S^2 familiar to the geometers, see e.g. [19],[20], [36]. The motivation of liquid crystals has generated a renewed interest in the study of *variational problems* involving vector-valued maps with *non-convex constraints* such as $u(x) \in S^2$. There are now many results concerning the energy (2) but very few results concerning the general energy (1). For simplicity I will deal here only with (2) and I refer the interested reader to the expository lecture of D. Kinderlehrer [31] for the general case.

As a conclusion to this introduction I would like to say the following :

1) I feel that the mathematical questions arising in this field are of great interest for their own sake, an interest which goes much beyond their connections to liquid crystals. However, the physical background provides a wonderful source of new mathematical problems and it suggests new tools to tackle them.

2) The mathematics involves an unusual combination of techniques from various fields such as, Nonlinear Partial Differential Equations, Functional Analysis, Differential Geometry, Geometry Measure Theory, Topology, Numerical Analysis, Graph Theory, etc.

The plan of the lecture is the following :

1. Minimal connections.
   1.1. New min-max principles.
   1.2. Minimizing the energy over maps with prescribed singularities.
   1.3. The dipole construction or How to create a pair of singularities.
   1.4. The D-field.
   1.5. Another approach via Federer's coarea formula.

2. Questions of density and nondensity for Sobolev maps between manifolds.
   2.1. Topology : an obstruction to density of smooth maps.
   2.2. A necessary and sufficient condition for the density of smooth maps.
   2.3. Density of maps with a finite number of singularities.
   2.4. Density for the weak topology. How to eliminate singularities.
   2.5. A characterization of maps which can be approximated by smooth maps.

3. Minimizing the energy E over all H^1 maps.
   3.1. $x/|x|$ is a minimizer.
   3.2. The singularities of minimizers.
   3.3. Energy estimates for maps which are odd on the boundary.

4. The gap phenomenon and relaxed energies for harmonic maps.
   4.1. The gap phenomenon.
   4.2. Relaxed energies for harmonic maps.

1. MINIMAL CONNECTIONS.

1.1. New min-max principles.

The notion of a minimal connection, introduced in [11], is a very convenient tool. In a metric space M, with distance d, suppose we have a family of "positive points" $p_1, p_2, ..., p_k$ and of "negative points" $n_1, n_2, ..., n_k$ (where some of these points may coincide). The length of a minimal connection is, by definition,

$$L = \min_{\sigma} \sum_{i=1}^{k} d(p_i\,,\, n_{\sigma(i)})$$

where the minimum is taken over all permutations σ of the integers $\{1, 2, ..., k\}$.

A useful formula for computing L is given by

THEOREM 1 ([11]).

$$L = \max_{\zeta \in \mathcal{L}} \{\sum_{i=1}^{k} \zeta(p_i) - \sum_{i=1}^{k} \zeta(n_i)\}$$

where

$$\mathcal{L} = \{\zeta : M \to \mathbb{R}; |\zeta(x) - \zeta(y)| \leq d(x, y) \quad \forall x, y \in M\}.$$

The proof of Theorem 1 (see [11]) relies on Kantorovich duality principle (see[35]) combined with Birkhoff's theorem on the extreme points of doubly stochastic matrices. A direct approach, in the spirit of linear programming, is given in [9].

Another development related to Theorem 1 is the following :

THEOREM 2 ([11]). *Let M be a compact metric space. Let μ be a probability measure on M. Then*

$$\min_{\nu\in\mathcal{A}} \max_{\zeta\in\mathcal{L}} \int \zeta\, d\mu - \zeta\, d\nu = \min_{y\in M} \int d(x,y)d\mu(x),$$

where $\mathcal{A}$ denotes the family of all measure ν of the form $\nu = \Sigma\, d_i\, \delta_{a_i}$ which are finite sums of Dirac masses with coefficients $d_i \in Z$ and $\Sigma\, d_i = 1$.

Theorem 2 is a new kind of min-max principle which does not seem to be related to any of the classical principles (Van Neumann, Ky-Fan, etc.), especially since $\mathcal{A}$ is not a convex set. An application of Theorem 2 is given in Section 3.1. It would be interesting to find applications in other areas (mathematical economics ?). The proof of Theorem 2 given in [9] is based on Theorem 1 and on a new combinatorial result of Hamidoune-Las Vergnas [27] conjectured by Coron-Lieb and myself :

LEMMA 1. *Let $\mathcal{G}$ be a graph which consists of p boys $B_1, B_2, ..., B_p$ and p girls $G_1, G_2, ..., G_p$, such that every boy is connected to m girls and every girl is connected to m boys (m and p are independent integers). Then, given any girl G_i there is some boy B_j which is connected to G_i by m disjoint (zigzagging) paths.*

1.2. Minimizing the energy over maps with prescribed singularities.

A natural question, originally raised by J. Ericksen, is to study the least deformation energy required to produce singularities at prescribed locations. This is a somewhat "academic" problem because one does not control physically the location of the singularities. However, it turns out that this problem has a very simple answer and it has stimulated the development of new techniques. For simplicity, we start with the (non realistic) case where the container Ω is all of $\mathbb{R}^3$. Fix N points $a_1, a_2, ..., a_N$ in $\mathbb{R}^3$ -the desired location of the singularities- and consider the class of all admissible maps :

$$\mathcal{E} = \{u \in C^1(\mathbb{R}^3 \setminus \bigcup_{i=1}^{N} \{a_i\}; S^2)\ ;\ \int_{\mathbb{R}^3} |\nabla u|^2 < \infty \text{ and } deg(u, a_i) = d_i \quad \forall i\}$$

where the d_i's are *given* integers, $d_i \in Z$, $d_i \neq 0$ and $deg(u, a_i)$ denotes the Brouwer degree of u restricted to any small sphere around a_i. The class $\mathcal{E}$ is nonempty iff $\Sigma\, d_i = 0$ and we shall make this assumption. Set

$$E = \inf_{u\in\mathcal{E}} \int |\nabla u|^2.$$

Surprisingly, there is an explicit formula for E :

THEOREM 3 ([11]). *$E = 8\pi L$ were L is the length of a minimal connection connecting the singularities.*

The precise definition of L is the following. The points (a_i) are relabelled as positive and negative points (p_i, n_i) which are repeated according to their multiplicity $|d_i|$. For example if $d_1 = +2$ we take $p_1 = p_2 = a_1$, etc. Since $\Sigma\, d_i = 0$, we have the same number of positive and negative points and then we use the definition of Section 1.1, with the euclidean distance,

$$L = \min_{\sigma} \Sigma\, |p_i - n_{\sigma(i)}|.$$

The proof of Theorem 3 is split into two independent steps.

Step 1 : $E \leq 8\pi L$,

Step 2 : $E \geq 8\pi L$.

Step 1 relies heavily on the dipole construction described in Section 1.3. Step 2 uses the notion of D-field introduced in Section 1.4 as well as Theorem 1 ; an alternative approach for Step 2, based on Geometric Measure Theory, is described in Section 1.5

There are two variants of Theorem 3 when $\mathbb{R}^3$ is replaced by a bounded domain Ω in $\mathbb{R}^3$.

Variant 1 (No boundary data). Fix N points $a_1, a_2, ..., a_N$ in Ω and consider the class

$$\mathcal{E}_1 = \{u \in C^1(\overline{\Omega} \setminus \bigcup_{i=1}^{N} \{a_i\}; S^2)\ ;\ \int_{\Omega} |\nabla u|^2 < \infty \text{ and } deg(u, a_i) = d_i \quad \forall i\}$$

As above we relabel the points (a_i) as positive and negative points. However we do *not* have to assume that $\Sigma\, d_i = 0$ and thus we need not have the same number of positive and negative points.

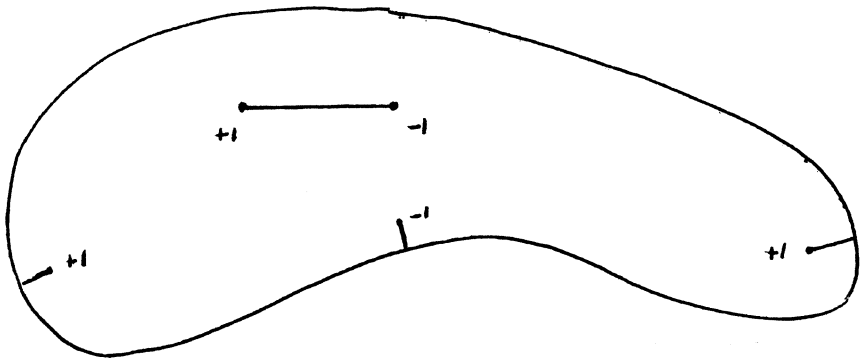
Set

$$E_1 = \inf_{u \in \mathcal{E}_1} \int |\nabla u|^2.$$

THEOREM 3_1. *$E_1 = 8\pi L_1$ where L_1 is the length of a minimal connection, allowing connections to the boundary.*

More precisely, each positive (resp. negative) point is connected *either* to a negative (resp. positive) point *or* to the boundary. Then, one takes the minimal length, L_1, over *all* such configurations

Example 1.



Variant 2 (Constant boundary data). Fix N points in Ω and consider the class

$$\mathcal{E}_2 = \{u \in \mathcal{E}_1 \ ; \ u \text{ is constant on } \partial\Omega\}.$$

Here we must assume that $\Sigma\, d_i = 0$ and thus we have the same number of positive and negative points.

Set

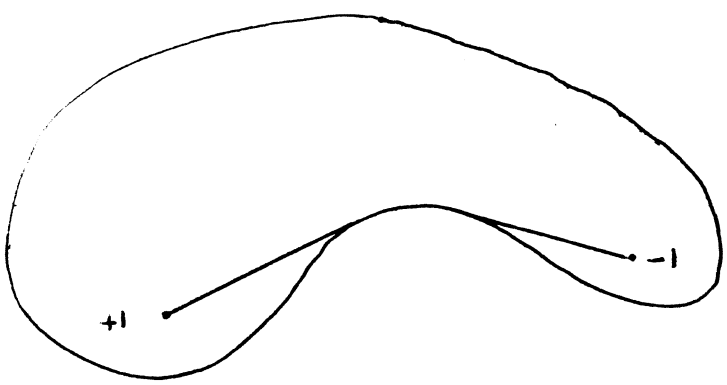
$$E_2 = \inf_{u \in \mathcal{E}_2} \int |\nabla u|^2.$$

THEOREM 3_2. *$E_2 = 8\pi L_2$ where L_2 is the length of a minimal connection relative to the geodesic distance d in $\overline{\Omega}$, i.e.*

$$L_2 = \min_{\sigma} \Sigma\, d(p_i\,,\, n_{\sigma(i)})$$

(Here connections to the boundary are not allowed).

Example 2.



Remark 1. The mysterious factor 8π is replaced by $2area(N)$ if S^2 is replaced by a 2-dimensional manifold N homeomorphic to S^2 (see [12]).

1.3. The dipole construction or How to create a pair of singularities.

The following construction is useful for various purposes :

THEOREM 4 ([11]). *Let p and n be two points in $\mathbb{R}^3$. Given any $\varepsilon > 0$ there is a map $u_\varepsilon : \mathbb{R}^3 \to S^2$ which is smooth everywhere except at p and n, such that :*

$$deg(u_\varepsilon, p) = +1 \quad , \quad deg(u_\varepsilon, n) = -1, \tag{3}$$

$$\int |\nabla u_\varepsilon|^2 \leq 8\pi|p-n| + \varepsilon \tag{4}$$

(5) *u_ε is constant outside an ε – neighborhood V_ε of the line segment $[p, n]$.*

For the proof of Theorem 4 we refer to [11] (or to [9]). The main idea is that u_ε "covers quickly" S^2 as one "crosses through" V_ε on a sphere around p, so that $|\nabla u_\varepsilon| \sim 1/\varepsilon$ in V_ε and $\int_{V_\varepsilon} |\nabla u_\varepsilon|^2 \sim (1/\varepsilon^2)(vol\, V_\varepsilon) \sim L$.

Gluing together these dipoles over a minimal connection it is easy to show that $E \leq 8\pi L$ in Theorem 3 (or 3_1). The proof of Theorem 3_2 requires the analogue of Theorem 4 where the line segment $[p, n]$ is replaced by a simple curve C going from p to n, $|p-n|$ is replaced by the length of C and V_ε is an ε tubular neighborhood of C.

1.4. The D-field.

To every map $u : \Omega \to S^2$ we associate the vector field $D : \Omega \to \mathbb{R}^3$ defined as follows

$$D = D(u) = (u \cdot u_y \times u_z \, , \, u \cdot u_z \times u_x \, , \, u \cdot u_x \times u_y)$$

where u_x , u_y , u_z denote the partial derivatives with respect to x, y, z. A more intrinsic way to define D is to consider the pull-back under u of the canonical 2-form on S^2. This vector field has some remarkable properties (see [11]) :

$$|D(u)| \leq \frac{1}{2} |\nabla u|^2 \quad \text{on } \Omega \tag{6}$$

and if $u \in C^1(\Omega \setminus \bigcup_{i=1}^N \{a_i\}; S^2)$, $\int_\Omega |\nabla u|^2 < \infty$,then

$$div D(u) = 4\pi \, \Sigma \, d_i \, \delta_{a_i} \quad \text{in } \mathcal{D}'(\Omega) \tag{7}$$

where $d_i = deg(u, a_i)$.

Formula (7) relies on the well-known analytic expression (see e.g. [34]) for the degree of a map $\varphi : S \to S^2$, mapping a 2-dimensional closed surface S into S^2,

$$deg\,\varphi = \frac{1}{4\pi}\int_S Jac\,\varphi\, d\sigma. \tag{8}$$

The D-field enters into the proof of Theorem 3 (Step 2) as follows. For $u \in \mathcal{E}$, write, using integration by parts,

$$\int_{\mathbb{R}^3} |\nabla u|^2 \geq 2\int_{\mathbb{R}^3} |D| \geq -2\int_{\mathbb{R}^3} D(u)\cdot\nabla\zeta = 2\int_{\mathbb{R}^3} [div D(u)]\zeta$$
$$= 8\pi\,\Sigma\, d_i\,\zeta(a_i)$$

for any function $\zeta : \mathbb{R}^3 \to \mathbb{R}$ such that $\|\nabla\zeta\|_{L^\infty(\Omega)} \leq 1$. Therefore, by Theorem 1,

$$\int |\nabla u|^2 \geq 8\pi \max_{\|\nabla\zeta\|_{L^\infty}\leq 1}\{\Sigma\, d_i\,\zeta(a_i)\} = 8\pi L.$$

For later purpose it is useful to keep in mind the following formulas which hold for all maps $u \in C^1(\overline{\Omega}\setminus\bigcup_{i=1}^N\{a_i\}; S^2)$ with $\int|\nabla u|^2 < \infty$ and provide estimates for the length of minimal connections in terms of the D-field. Let $L_1(u)$ be the length of the minimal connection, connecting the singularities of u and *allowing connections to the boundary*. It is easy to see, using Theorem 1, that

$$L_1(u) = \max_\zeta\{\Sigma\, d_i\,\zeta(a_i)\,;\ \|\nabla\zeta\|_{L^\infty(\Omega)} \leq 1 \text{ and } \zeta = 0 \text{ on } \partial\Omega\}.$$

It follows that

$$L_1(u) = \frac{1}{4\pi}\max_\zeta\{\int D(u)\cdot\nabla\zeta\,;\ \|\nabla\zeta\|_{L^\infty(\Omega)} \leq 1 \text{ and } \zeta = 0 \text{ on } \partial\Omega\} \tag{9}$$

and in particular

$$L_1(u) \leq \frac{1}{8\pi}\int |\nabla u|^2. \tag{10}$$

Assuming in addition that $deg\, u_{|\partial\Omega} = 0$, then $\Sigma\, d_i = 0$ and we may consider $L_2(u)$, the length of a minimal connection relative to the *geodesic distance* in $\overline{\Omega}$ (and excluding connections to $\partial\Omega$). Then, $L_2(u) = \max\{\Sigma\, d_i\,\zeta(a_i)\,;\ \|\nabla\zeta\|_{L^\infty(\Omega)} \leq 1\}$ and therefore

$$L_2(u) = \frac{1}{4\pi}\max_\zeta\{\int_\Omega D(u)\cdot\nabla\zeta - \int_{\partial\Omega} D(u)\cdot n\,\zeta\,;\ \|\nabla\zeta\|_{L^\infty(\Omega)} \leq 1\}. \tag{11}$$

1.5. Another approach via Federer's coarea formula.

An interesting alternative proof for Theorem 3, Step 2, has been found by F. Almgren - W. Browder - E. Lieb (see [2]). It relies heavily on Federer's coarea formula, which we recall for convenience. Suppose u is a C^1 map from a domain $\Omega \subset \mathbb{R}^n$ with values into a manifold N of dimension $p \leq n$. Its differential Du is a $(p \times n)$ matrix. Set

$$J_p\, u = \sqrt{det(Du \cdot (Du)^t)}.$$

The coarea formula says that

$$\int_\Omega J_p\, u\, dx = \int_\Omega \mathcal{H}^{n-p}(u^{-1}(\sigma))d\sigma$$

where $\mathcal{H}^{n-p}$ is the $(n-p)$-dimensional Hausdorff measure in $\mathbb{R}^n$. In the case of interest to us we take $u \in \mathcal{E}$, $\Omega = \mathbb{R}^3 \setminus \cup\{a_i\}$ and $N = S^2$; we are led to

$$\int_{\mathbb{R}^3} J_2\, u\, dx = \int_{S^2} \mathcal{H}^1(u^{-1}(\sigma))d\sigma.$$

It is easy to see that

$$J_2\, u \leq \frac{1}{2}\,|\nabla u|^2$$

and therefore

$$\int_{\mathbb{R}^3} |\nabla u|^2 \geq 2 \int_{S^2} \mathcal{H}^{-1}(\sigma))d\sigma.$$

To obtain the conclusion of Theorem 3 (Step 2) it suffices to know that, for a.e. $\sigma \in S^2$,

$$\mathcal{H}^1(u^{-1}(\sigma)) \geq L. \tag{12}$$

Sard's theorem implies that a.e. $\sigma \in S^2$ is a regular value and then $u^{-1}(\sigma)$ is a collection of curves which either connect two singularities or go to infinity or are closed loops. $\mathcal{H}^1(u^{-1}(\sigma))$ is the total length of these curves. One proves (see e.g. [10]) that this collection of curves must include a disjoint union of (zigzagging) paths connecting each p_i to $n_{\sigma(i)}$ for some permutation σ and then (12) follows.

2. QUESTIONS OF DENSITY AND NONDENSITY FOR SOBOLEV MAPS BETWEEN MANIFOLDS.

Let Ω be a smooth domain in $\mathbb{R}^n$ or more generally and n-dimensional manifold (with or without boundary). Let N be a compact manifold without boundary embedded in $\mathbb{R}^k$. As usual the Sobolev space $W^{1,p}$, for $1 \leq p < \infty$, is defined by

$$W^{1,p}(\Omega;\mathbb{R}^k) = \{u \in L^p(\Omega;\mathbb{R}^k)\,;\ \nabla u \in L^p\}$$

and one writes H^1 for $W^{1,2}$.

Set

$$W^{1,p}(\Omega;N) = \{u \in W^{1,p}(\Omega;\mathbb{R}^k)\,;\ u(x) \in N \text{ a.e.}\}.$$

It is well-known (see e.g. [1]) that smooth maps $C^\infty(\overline{\Omega};\mathbb{R}^k)$ are dense in $W^{1,p}(\Omega;\mathbb{R}^k)$ and it is natural to raise (see Eells - Lemaire [19]) the

Question : Is $C^\infty(\overline{\Omega};N)$ dense in $W^{1,p}(\Omega;N)$?

If $p > n = dim\,\Omega$, the Sobolev embedding theorem asserts that $W^{1,p} \subset C^0$. Using this fact and standard smoothing methods it is easy to see that the answer is *yes*. When $p = n$ the same conclusion still holds, but the argument is slightly more complicated (see Schoen - Uhlenbeck [38]).

We are left with the interesting case $p < n$.

2.1. Topology : an obstruction to density of smooth maps.

The following striking example, due to Schoen - Uhlenbeck [38] shows that the answer may sometimes be *negative*.

Let $\Omega = B^3 = \{x \in \mathbb{R}^3\,;\ |x| < 1\}$ and let $N = S^2$. Then

$$C^\infty(\overline{\Omega};S^2) \text{ is } \textit{not} \text{ dense in } H^1(\Omega;S^2).$$

In fact set

$$u(x) = \frac{x}{|x|},$$

so that $u \in H^1(\Omega;S^2)$. We claim that there is no sequence $u_j \in C^\infty(\overline{\Omega};S^2)$ such that $u_j \to u$. Suppose, by contradiction, that such a sequence exists. Then for a.e. sphere S_r (centered at 0, of radius r)

$$u_{j|S_r} \to u_{|S_r} \text{ in } H^1(S_r). \tag{13}$$

On the one hand,

$$deg(u_{j|S_r}) = 0 \tag{14}$$

because u_j has a smooth extension inside B_r. On the other hand, since $u(x) = x/|x|$,

$$deg(u_{|S_r}) = 1. \tag{15}$$

We obtain a contradiction from (13), (14) and (15) if we know that the degree is continuous under H^1 convergence ; this is a consequence of the representation formula (8).

2.2. A necessary and sufficient condition for the density of smooth maps.

The above question has been beautifully settled by Bethuel [4], [6] (see also the earlier work of Bethuel - Zheng [8]). The answer involves some *homotopy group* of N :

THEOREM 5. *Assume $1 \leq p < n$. Then $C^\infty(\overline{\Omega}; N)$ is dense in $W^{1,p}(\Omega; N)$ iff $\pi_{[p]}(N) = 0$.*

If $\pi_{[p]}(N) \neq 0$ one constructs explicity a map $u \in W^{1,p}(\Omega; N)$ which can not be approximated by smooth maps. The idea is the same as in Section 2.1, except that instead of using the continuity of the degree one uses the fact (see [40]) that some homotopy classes are closed under Sobolev convergence.

The proof of the converse, i.e. $\pi_{[p]}(N) = 0$ implies density, is very delicate. Any map $u \in W^{1,p}$ is first approximated by maps which are smooth except on "small sets". This is done without any assumption on N (see Section 2.3). Next, these singularities are "removed" using the assumption $\pi_{[p]}(N) = 0$.

Example : $\Omega \subset \mathbb{R}^3$, $N = S^2$,

$$\begin{cases} 1 \leq p < 2 : \text{Density}, \\ 2 \leq p < 3 : \text{No density}, \\ 3 \leq p < \infty : \text{Density}. \end{cases}$$

2.3. Density of maps with a finite number of singularities.

In the case where smooth maps are not dense it is useful to have another class of "decent" maps which is dense. Here is a typical example which has many applications. Let $\Omega \subset \mathbb{R}^3$ be a smooth domain and let N be any manifold without boundary.

Set

$$R = \{u \in H^1(\Omega; N) | u \text{ is smooth on } \overline{\Omega} \text{ except at a finite number of points}\}$$

(there is no restriction on the number or the location of the singularities).

THEOREM 6 ([6], [8]). *R is dense in $H^1(\Omega; N)$.*

In the case where $N = S^2$ there is a rather simple proof of Theorem 6. The idea is the following. Fix $u \in H^1(\Omega; S^2)$ and let (v_j) be a sequence in $C^\infty(\overline{\Omega}; B^3)$ such that $v_j \to u$ in H^1. Given $a \in B^3$, let P_a be the radial projection with vortex at a from B^3 onto S^2. Set $u_j = P_a(v_j)$. Sard's theorem and a device of Hardt-Lin (see [30]) show that for a.e. a, $u_j \in R\ \forall j$ and $u_j \to u$ in H^1. This kind of argument seems to be restricted to $N = S^2$ and it would be interesting to have a simple proof for a general manifold N.

Remark 2. The general form of Theorem 6 is the following (see [6]). Assume $\Omega \subset \mathbb{R}^n$ and let $1 \leq p < n$. Set

$$R = \{u \in W^{1,p}(\Omega; N)\,;\ u \text{ is smooth on } \overline{\Omega} \text{ except on a set of dimension } n - [p] - 1\}.$$

Then R is dense in $W^{1,p}(\Omega; N)$.

Remark 3. The same kind of result holds with boundary conditions. For example let $g : \partial\Omega \to N$ be a smooth map. Set

$$H^1_g(\Omega; N) = \{u \in H^1(\Omega; N)\,;\ u = g \text{ on } \partial\Omega\}$$

and

$$R_g = \{u \in R\,;\ u = g \text{ on } \partial\Omega\}.$$

Then R_g is dense in $H^1_g(\Omega; N)$.

2.4. Density for the weak topology. How to eliminate a pair of singularities.

In the case where smooth maps are *not* dense for the strong $W^{1,p}$ topology, one may ask whether they are dense for the weak $W^{1,p}$ topology. There are some partial results in this direction. For simplicity we shall assume here that $\Omega \subset \mathbb{R}^3$ and $N = S^2$.

THEOREM 7 ([6]). *Given any $u \in H^1(\Omega; S^2)$ there is a sequence (u_j) in $C^\infty(\overline{\Omega}; S^2)$ such that $u_j \rightharpoonup u$ weakly in H^1.*

Remark 4. The same conclusion *fails* for $W^{1,p}$ with $2 < p < 3$. One may use the same kind of argument as in Section 2.1.

The proof of Theorem 7 relies on the following important construction due to Bethuel [5] which may be considered as the "reverse" operation of the dipole construction.

THEOREM 8. *(How to eliminate a pair of singularities). Let $v \in H^1(\Omega; S^2)$ be smooth on $\overline{\Omega}$ except at two points (p, n) such that $deg(v, p) = +1$, $deg(v, n) = -1$ and the line segment $[p, n]$ is contained in Ω.*

Then, given any $\varepsilon > 0$, there is a map $v_\varepsilon : \overline{\Omega} \to S^2$ which is smooth everywhere on $\overline{\Omega}$ and

$$v_\varepsilon = v \text{ outside an } \varepsilon\text{-neighborhood } V_\varepsilon \text{ of the line segment } [p, n] \tag{16}$$

$$\int_\Omega |\nabla v_\varepsilon|^2 \leq \int_\Omega |\nabla v|^2 + 8\pi|p - n| + \varepsilon. \tag{17}$$

In other words, it is possible to remove a pair of singularities (p, n) without changing "too much" the original map, but the price to pay is an increase in energy of the order $8\pi|p - n|$.

Here are two useful variants of Theorem 8 :

Variant 1 : The line segment $[p, n]$ is replaced by a simple curve C in Ω going from p to n, $|p - n|$ is replaced by the length of C and V_ε is an ε tubular neighborhood of C.

Variant 2 : One can also eliminate a singularity "towards the boundary". Suppose, for example, $v \in H^1(\Omega; S^2)$ is smooth except on $\overline{\Omega}$ at one point p with $deg(v, p) = +1$. Let $n \in \partial\Omega$ be such that $|p - n| = dist(p, \partial\Omega)$. Then given any $\varepsilon > 0$ there is a map $v_\varepsilon : \overline{\Omega} \to S^2$ which is smooth *everywhere* on $\overline{\Omega}$ satisfying (16) and (17). [This construction however changes the boundary value of v].

We may now return to Theorem 7. Given $u \in H^1(\Omega; S^2)$, there is (by Theorem 6) a sequence $v_j \in R$ such that $v_j \to u$ in H^1. One eliminates the singularities of each v_j using Theorem 8 (or its Variant 2). Choosing an optimal pairing of the singularities (or connecting them to $\partial\Omega$), the increase in energy is at most $8\pi L_1(v_j)$ (defined in Section 2.2). On the other hand, by (10), $L_1(v_j) \leq 1/8\pi \int |\nabla v_j|^2$ and thus we may find a sequence (w_j) in $C^\infty(\overline{\Omega}; S^2)$ such that $w_j \to u$ a.e. and $\limsup \int |\nabla w_j|^2 \leq 2 \int |\nabla u|^2$. It follows that $w_j \rightharpoonup u$ weakly in H^1.

Remark 4. We may also preserve the boundary condition. Assume, for example $g : \partial\Omega \to S^2$ is a smooth map with $deg(g, \partial\Omega) = 0$. Given any $u \in H^1(\Omega; S^2)$ with $u = g$ on $\partial\Omega$ there is a sequence (u_j) in $C^\infty(\overline{\Omega}; S^2)$ with $u_j = g$ on $\partial\Omega$ such that $u_j \rightharpoonup u$ weakly in H^1 [The proof relies on Variant 1 and formula (11)].

2.6. A characterization of maps which can be approximated by smooth maps.

In the case where smooth maps are not dense it is natural to ask whether a *given* map u can be approximated by smooth maps strongly in $W^{1,p}$. Here is an interesting criterion due to Bethuel [5] for $\Omega \subset \mathbb{R}^3$ and $N = S^2$.

THEOREM 9. *Let $u \in H^1(\Omega; S^2)$. Then there exists a sequence $u_j \in C^\infty(\overline{\Omega}; S^2)$ such that $u_j \to u$ in H^1 iff $div\, D(u) = 0$ in the sense of distributions.*

The proof of Theorem 9 relies on Theorem 6 and on the technique of elimination of singularities describes in Section 2.5.

3. MINIMIZING THE ENERGY OVER ALL H^1 MAPS.

Let $\Omega \subset \mathbb{R}^3$ be a smooth bounded domain and let $g : \partial\Omega \to S^2$ be a smooth boundary data. Consider the problem of minimizing the energy over the class of *all* H^1 maps from Ω into S^2 with boundary data g. Clearly

$$\inf_{H^1_g(\Omega;S^2)} \int |\nabla u|^2 \tag{18}$$

is achieved. Any minimizer satisfies the corresponding Euler equations

$$-\Delta u = u|\nabla u|^2 \tag{19}$$

which is the equation of harmonic maps (see e.g. [19]). This equation is satisfied in the weak sense of distributions. Note that (19) is not a scalar equation but a *system*. The regularity of solutions of elliptic systems is a delicate matter (see e.g. [18], [26], [24]), especially when they involve $|\nabla u|^2$. In general one has only *partial* regularity results, i.e. minimizers are smooth except on closed sets of low dimension. In our case, a result of Schoen-Uhlenbeck [37],[38] asserts that every *minimizer* u of (18) is *smooth except at a finite number of points*. In contrast with Section 1.2 the number and the location of the singularities is not given in advance. Singularities are free to appear wherever they want as long as they "help" to lower the energy. In Section 3.2 I will describe some properties of these singularities. If $deg(g, \partial\Omega) \neq 0$ there is a *topological obstruction* to regularity since g cannot be extended smoothly inside Ω. However, if $deg(g, \partial\Omega) = 0$ there is *no topological obstruction* to regularity since g can be extended smoothly inside Ω. Nevertheless singularities may occur. This phenomenon will be discussed in Section 4.

3.1. $x/|x|$ is a minimizer.

We start with a simple question. Let $\Omega = B^3$ and let $g(x) = x$ be the identity map on $\partial\Omega$.

THEOREM 10 ([11]). *The map $u(x) = x/|x|$ is a minimizer for (18). In fact, it is the unique minimizer.*

I will sketch a proof based on the D-field approach. Since

$$\int_\Omega |\nabla(\frac{x}{|x|})|^2) = 8\pi$$

it suffices to prove that

$$\int |\nabla u|^2 \geq 8\pi \qquad \forall u \in H^1_g(\Omega; S^2). \tag{20}$$

In view of Remark 3 we may assume that $u \in R_g$. We have

$$\int_\Omega |\nabla u|^2 \geq 2\int_\Omega |D(u)| \geq 2\int_\Omega D(u)\cdot\nabla\zeta \tag{21}$$

for any function $\zeta : \Omega \to \mathbb{R}$ such that $\|\nabla\zeta\|_{L^\infty} \leq 1$. Integrating by parts we find

$$\int_\Omega D(u)\cdot\nabla\zeta = \int_{\partial\Omega} D(u)\cdot n\,\zeta\,d\sigma - \int_\Omega (div\,D(u))\zeta. \tag{22}$$

It easy to check that $D(u)\cdot n = 1$ on $\partial\Omega$ (since $u(x) = x$ on $\partial\Omega$). On the other hand (see (7))

$$div\,D(u) = 4\pi\Sigma\, d_i\,\delta_{a_i} \tag{23}$$

Thus, by (21), (22), (23)

$$\int_\Omega |\nabla u|^2 \geq 8\pi\,\{\int \zeta\,d\mu - \int \zeta\,d\nu\}$$

where $d\mu = (1/4\pi)\,d\sigma$ is the surface measure on S^2 and $d\nu = \Sigma\, d_i\,\delta_{a_i}$ with $\Sigma\, d_i = 1$ since g has degree one on $\partial\Omega$. Using the notations of Theorem 2 we have

$$\int_\Omega |\nabla u|^2 \geq 8\pi \min_{\nu\in\mathcal{A}}\max_{\zeta\in\mathcal{L}}\{\int \zeta\,d\mu - \int \zeta d\nu\}.$$

By Theorem 2, $RHS = 8\pi \min_{y\in\overline{\Omega}} \int_{S^2} |y-\sigma|\,d\sigma/4\pi = 8\pi$.

Remark 5. There is another proof of F.H. Lin [33] (see also [10]) for Theorem 10 which extends to n-dimensions (B^3 is replaced by B^n and S^2 is replaced by S^{n-1}.

3.2. The singularities of minimizers.

The first result concerns the asymptotic behavior of a minimizer u near a singularity :

THEOREM 11 ([11]). *Assume $\Omega \subset \mathbb{R}^3$ is any domain and $g : \partial\Omega \to S^2$ is any boundary data. Let u be a minimizer for (18) and let x_0 be a singularity of u. Then there is a rotation R such that*

$$y(x) \simeq \pm \frac{R(x - x_0)}{|x - x_0|} \quad \text{as} \quad x \to x_0.$$

In particular, every singularity has degree ± 1.

Remark 6. Prior to this result, Hardt-Kinderlehrer-Lin [28] had obtained a universal bound for the degree of singularities. Experimental and numerical evidence (see [13] and [15]) suggested that this degree is ± 1.

The proof of Theorem 11 relies on a *blow-up technique* originally introduced in [26] and on a careful analysis of the *homogeneous tangent maps*. Taking $x_0 = 0$, $u(\varepsilon x) \to \psi(x)$ as $\varepsilon \to 0$ (see [37] and [39]), where ψ is a minimizing harmonic map depending only on the direction $x/|x|$, say $\psi(x) = h(x/|x|)$. A crucial ingredient is the following lemma whose proof is quite involved :

LEMMA 2 ([11]). *Assume $\Omega = B^3$ and $h : \partial\Omega \to S^2$ is any boundary data. Then the homogeneous extension $\psi(x) = h(x/|x|)$ is not a minimizer unless h is a constant or $h = \pm$ Rotation (the latter case corresponds to Theorem 10).*

A challenging question is to estimate the *number of singularities*. A major achievement in this direction is the following :

THEOREM 12 ([3]). *The number of singularities bounded by $C \int_{\partial\Omega} |\nabla_T g|^2 \, d\sigma$ (where ∇_T denotes the tangential gradient), for some constant C.*

Remark 7. The proof Theorem 12 is quite involved and there is no explicit control on the constant C. For example, it would be interesting to know whether the condition $\int_{\partial\Omega} |\nabla_T g|^2 < 8\pi$ implies that any minimizer has no singularity.

3.3. Energy estimates for maps which are odd on the boundary.

The following result conjectured in [11] is due to Coron-Gulliver [16] :

THEOREM 13. *Assume $\Omega = B^3$ and let $g = \partial\Omega \to S^2$ be an odd boundary data, i.e. $g(-x) = -g(x)$ on $\partial\Omega$. Then*

$$\int_\Omega |\nabla u|^2 \geq 8\pi \qquad \forall u \in H^1_g(\Omega; S^2).$$

In particular, if $g(x) \equiv x$ we obtain that $x/|x|$ is a minimizing harmonic map (Theorem 10). The proof of Theorem 13 relies on a combination of the coarea formula as in Section 1.5 and Borsuk's theorem (the degree of an odd map is odd) ; see also [10].

Remark 8. The n-dimensional extension of Theorem 13 is not known. More precisely, assume $u \in H^1(B^n; S^{n-1})$ is odd on ∂B^n ; does one have

$$\int_{B^n} |\nabla u|^2 \geq \int_{B^n} |\nabla(\frac{x}{|x|})|^2 \,?$$

4. THE GAP PHENOMENOM AND RELAXED ENERGIES FOR HARMONIC MAPS.

4.1. The gap phenomenon.

This is a very intriguing phenomenon originally discovered by Hardt-Lin [29]. A simpler example of the same phenomenon is given in [9].

THEOREM 14. *Let Ω be any smooth bounded domain in $\mathbb{R}^3$. There exists a smooth boundary data $g : \partial\Omega \to S^2$, of degree zero, such that*

$$\min_{u \in H^1_g(\Omega; S^2)} \int |\nabla u|^2 < \inf_{\substack{u \in C^1(\overline{\Omega}; S^2) \\ u = g \text{ on } \partial\Omega}} \int |\nabla u|^2 \tag{24}$$

For such a g any minimizer of (18) *must* have singularities. This is an example where *it "pays" for the system to create singularities in order to lower its energy.* The construction of g involves two dipoles (in the sense of Section 1.3) and the proof of (24) relies on a D-field argument.

Remark 9. By choosing appropriate g's one can make the LHS in (24) smaller than any given ε and the RHS larger than any given number.

It is a *major open problem* to decide whether, for every smooth g with $deg(g, \partial\Omega) = 0$,

$$\inf_{\substack{u \in C^1(\overline{\Omega}; S^2) \\ u = g \text{ on } \partial\Omega}} \int |\nabla u|^2 \tag{25}$$

is achieved. In the next section we discuss an attempt to solve this problem. If the infimum (25) is achieved it would give a *smooth* harmonic map u such that $u = g$ on $\partial\Omega$. The existence of such a map is already an open problem. A minimizer for (25) could be of physical interest. In some experiments on liquid crystals, physicists (P. Cladis, personal communication) observe first a configuration with two point defects (of opposite sign). After a few days the defects move towards each other and eventually they annihilate. This suggests that the final configuration -which is smooth- corresponds to a minimizer of (25).

4.2. Relaxed energies for harmonic maps.

Let $\Omega \subset \mathbb{R}^3$ be any smooth bounded domain and let $g : \partial\Omega \to S^2$ be a smooth boundary data with $deg(g, \partial\Omega) = 0$. For simplicity we write H^1_g instead of $H^1_g(\Omega; S^2)$. Recall that

$$R_g = \{u \in H^1_g \,;\, u \text{ is smooth on } \overline{\Omega} \text{ except at a finite number of points}\}$$

is dense in H^1_g. For $u \in R_g$, $L_2(u)$ denotes (as in Section 1) the length of a minimal connection relative to the geodesic distance in Ω and excluding connections to the boundary. Observe that we have the same number of positive and negative points since $deg(g, \partial\Omega) = 0$ implies $\Sigma\, d_i = 0$.

Recall formula (11) :

$$L_2(u) = \frac{1}{4\pi} \max_{\zeta} \{ \int_\Omega D(u) \cdot \nabla\zeta - \int_{\partial\Omega} D(u) \cdot n\, \zeta \,;\, \|\nabla\zeta\|_{L^\infty(\Omega)} \leq 1\}$$

Note that $D(u) \cdot n = Jac\, g$ on $\partial\Omega$ (the 2×2 Jacobian determinant of g on $\partial\Omega$) and thus $\int_{\partial\Omega} D(u) \cdot n = 4\pi\, deg(g, \partial\Omega) = 0$; this implies that $L_2(u) < \infty$.

It is a remarkable fact that $L_2(u)$ *makes sense* -through (11)- for *any* map $u \in H^1_g$ and moreover one has

LEMMA 3 ([7]). *There is a constant C such that*

$$|L_2(u) - L_2(v)| \leq C\|u - v\|_{H^1}(\|u\|_{H^1} + \|v\|_{H^1}) \quad \forall u, v \in H^1_g.$$

In other words, the length of a minimal connection defined first for $u \in R_g$ extends by continuity to H^1_g. The following expression, defined for every $u \in H^1_g$,

$$E^*(u) = \int |\nabla u|^2 + 8\pi\, L_2(u)$$

seems to play an important role. Its main properties are collected in

THEOREM 15 ([7]).

(a) *E^* is lower semi-continuous for the weak topology on H^1_g and in particular*

$$\min_{u \in H^1_g} E^*(u) \tag{26}$$

is achieved.

$$\min_{u \in H^1_g} E^*(u) = \inf_{\substack{u \in C^1(\overline{\Omega}; S^2) \\ u = g \text{ on } \partial\Omega}} \int |\nabla u|^2. \tag{b}$$

(c) *E^* is a relaxed energy in the sense that, for every $u \in H^1_g$,*

$$E^*(u) = \inf\{\liminf \int |\nabla v_n|^2 \mid v_n \in C^1(\overline{\Omega}); S^2), v_n = g \text{ on } \partial\Omega \text{ and } v_n \rightharpoonup u \text{ weakly in } H^1\}$$

where the infimum is taken over all admissible sequences (v_n) (see Theorem 7 and Remark 4).

d) *Any minimizer u^* for (26) satisfies*

$$-\Delta u^* = u^*|\nabla u^*|^2 \text{ in the sense of distributions.}$$

The proof Theorem 15 relies heavily on Theorem 8 (and its Variant 1). The consequences of Theorem 15 are the following :

A. If the infimum in (25) is achieved by some u, then u is a minimizer for E^* on H^1_g

B. If u^* is a minimizer for E^* on H^1_g (we know it exists !) and if *in addition* u^* is smooth then u^* is a minimizer for (25).

Thus we have replaced the original problem of *existence* in (25) by a weaker problem which always admits a solution. The major open problem (a non trivial one !) is now a question of *regularity*. In any case -whether the minimizers of E^* are smooth or not- we have produced a *new harmonic map* which is not an absolute minimizer of E. One can prove (see [7]) that as soon as a gap occurs (i.e. (24) holds) the set of minimizers for E and E^* on H^1_g are disjoint.

This approach suggests that there are many "energies" associated with harmonic maps, not just $\int |\nabla u|^2$. Using this idea one can prove, for example, the following

THEOREM 16 ([7]). *Let $\Omega \subset \mathbb{R}^3$ be any smooth bounded domain and let $g : \partial\Omega \to S^2$ be any smooth boundary data which is not a constant. Then there exist infinitely many harmonic maps such that $u = g$ on $\partial\Omega$.*

These harmonic maps are just H^1 maps satisfying (19) in the sense of distributions. We have no information about their regularity.

Remark 10. Motivated by Cartesian currents, Giaquinta - Modica - Soucek [25] have also been led to the introduction of some kind of relaxed energy.

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