LIQUID CRYSTALS AND ENERGY ESTIMATES FOR S^2-VALUED MAPS

BY

HAÏM BREZIS

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Haïm Brezis

Département de Mathématiques
Université Paris VI
4 Pl. Jussieu
75252 Paris Cedex 05

This report summarizes results obtained in collaboration with J.M. Coron and E. Lieb (see [3] and [4]); it answers some questions raised by J. Ericksen and D. Kinderlehrer. The original motivation comes from the theory of liquid crystals (see [7], [8], [10]), and is well explained in other contributions to this volume.

We deal with maps ϕ from a domain Ω R^3 with values into S^2 which admit a finite number of singularities. We consider two different kinds of problems. In the first type of problem the location and the degree of the singularities is prescribed; the main result is an explicit formula, when $\Omega = R^3$, for the minimum value of the deformation energy. In the second type of problem the number, the location and the degree of the singularities are "free"; our main result asserts that if ϕ is a minimizer then all its singularities have degree ± 1, moreover, the first order expansion shows that ϕ (or $-\phi$) acts like a rotation near every singularity - a fact which agrees with experimental and numerical evidence (see [5] and [6]).

1. Prescribed Singularities

Fix N points $a_1, a_2, \ldots a_N$ in R^3 (the desired location of the singularities). Consider maps ϕ which are smooth on $R^3 \quad \bigcup_{i=1}^{N} \{a_i\}$, with values in S^2, and with finite energy, i.e.

$$E(\phi) = \int_{R^3} |\nabla\phi|^2 < \infty$$

[The most general energy of interest in the theory of liquid crystals is

$$\tilde{E}(\phi) = K_1 \int (\operatorname{div}\phi)^2 + K_2 \int |\phi\cdot\operatorname{curl}\phi|^2 + K_3 \int |\phi\wedge \operatorname{curl}\phi|^2$$

which is equivalent to $E(\phi)$ when $K_1 = K_2 = K_3 = 1$; it is an interesting open problem to extend our results to $\tilde{E}$] .

The fact that $E(\phi) < \infty$ does not imply that ϕ is continuous at the points a_i . A typical example of a ϕ with a singularity at $x = 0$ and locally finite energy is $\phi(x) = x/|x|$.

The degree of ϕ at a_i , $\deg(\phi,a_i)$, is defined to be the (Brouwer) degree of ϕ restricted to any small sphere around a_i . The class of <u>admissible maps</u> consists of

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

where the d_i' s are <u>given</u> integers (positive or negative). [Experimental evidence shows that the only observed degrees are ± 1 and the reason will be explained in Section 2 ; but, a priori, it makes mathematical sense to consider all possible integers].

Note that if the class $\mathcal{E}$ of admissible maps is not empty, then we must have

$$\sum_{i=1}^{N} d_i = 0 \tag{1}$$

because the assumption $\int_{\mathbb{R}^3} |\nabla\phi|^2 < \infty$ implies that, in some weak sense, ϕ tends to a constant at infinity and therefore the total degree must be zero. Conversely, if (1) holds, then $\mathcal{E}$ is not empty (this follows from the construction below).

Our purpose is to investigate the least deformation energy E needed to produce singularities of assigned degree at a prescribed location, namely,

$$E = \inf_{\phi \in \mathcal{E}} \int |\nabla\phi|^2 \quad . \tag{2}$$

The main results of Section 1 are the following:

Theorem 1 $$E = 8\pi L$$

where L is the length of a minimal connection (a notion which will defined later).

Theorem 2 The infimum in (2) is <u>not</u> achieved. If (ϕ_n) denotes a minimizing sequence, then there is a subsequence (ϕ_{n_k}) which converges to a constant a.e. and such that $|\nabla\phi_{n_k}|^2$ converges in the sense of measures to $8\pi\ \delta_C$ where C is some minimal connection and δ_C is the one-dimensional Hausdorff measure uniformly distributed over C.

In order to explain the concept of a minimal connection it is convenient to consider first some simple cases:

Example 1. The system consists only of two points a_1, a_2 with degrees $+1$ and -1. This basic example will be called a <u>dipole</u>. Here, $L = |a_1 - a_2|$ is the distance between the two points and δ_C is the uniform one-dimensional Hausdorff measure of the segment $[a_1,a_2]$. It is not surprising, from dimensional analysis, that E has the homogeneity of a length.

Example 2 The system consists of many points (a_i) and all the degrees d_i's are ± 1. Because of assumption (1) there are as many pluses as minuses. We relabel the points (a_i) by distinguishing the positive points $p_1, p_2 \ldots p_k$ and the negative points $n_1, n_2 \ldots n_k$.

Here,

$$(3) \qquad L = \operatorname*{Min}_{\sigma} \sum_{i=1} |p_i - n_{\sigma(i)}|$$

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

A minimal connection is, by definition, a union of segments

$$C = \bigcup_{i=1}^{k} [p_i, n_{\sigma(i)}]$$

where σ is a minimizing permutation in (3). There may be several minimal connections.

Theorem 2 says that if (ϕ_n) is a minimizing sequence, then all its energy tends to "concentrate" near some minimal connection.

Example 3 . In the general case where the d_i's are any integers one proceeds as in Example 2 except that the points a_i are repeated according to their multiplicity $|d_i|$.

Remark 1 There are variants of Theorem 1 when R^3 is replaced by a domain Ω and the class of admissible maps consist either of

$$\mathcal{E}_1 = \{\phi \in C^1(\Omega \setminus \bigcup_{i=1}^{k} \{a_i\};\ S^2) \mid \int_\Omega |\nabla\phi|^2 < \infty\ ,\ \deg(\phi, a_i) = d_i\}$$

or of

$$_2 = \{\phi \in C^1(\overline{\Omega} \setminus \bigcup_{i=1}^{k} \{a_i\};\ S^2) \mid \int_\Omega |\nabla\phi|^2 < \infty\ ,\ \deg(\phi, a_i) = d_i \text{ and } \phi \text{ is constant on } \partial\Omega\}.$$

For example, in the latter case the formula is

$$E_2 = \operatorname*{Inf}_{\rho \in \mathcal{E}_2} \int |\nabla\phi|^2 = 8\pi\, L_2$$

where

$$L_2 = \operatorname*{Min}_{\sigma} \sum_{i=1}^{k} d_\Omega\,(p_i\ ,\ n_{\sigma(i)})$$

and $d_\Omega(p,n)$ denotes the geodesic distance between p and n <u>within</u> Ω (see [4]).

<u>Remark 2</u> One may conceive of other problems where the <u>energy has the homogeneity of an area</u>. Consider, for example, a fixed Jordan curve Γ in $\mathbb{R}^3$. The class of admissible maps consists of

$$\mathcal{E} = \{\phi \in C^1(\mathbb{R}^3 \setminus \Gamma;\ S^1) \mid \int_{\mathbb{R}^3} |\nabla\phi| < \infty \text{ and } \deg(\phi, \Gamma) = 1\},$$

where $\deg(\phi,\Gamma)$ is the circulation of ϕ around Γ i.e. the degree of ϕ restricted to any circle which links with Γ. The energy

$$E(\phi) = \int_{\mathbb{R}^3} |\nabla\phi|$$

has the dimension of an area (instead of a length).

We conjecture that

$$E = \operatorname*{Inf}_{\phi \in \mathcal{E}} \int |\nabla\phi| = 2\pi A \tag{4}$$

where A is the area of an area - minimizing surface spanned by Γ. (Formula (4) is established in the case where Γ is a planar curve, see [4]). This is just the analogue of the dipole formula. One may imagine a similar problem for a collection of oriented curves (Γ_i), the class of admissible maps being

$$E = \{\phi \in C^1(R^3 \setminus \bigcup_{i=1}^{k} \Gamma_i ; S^1) \mid \int |\nabla\phi| < \infty \text{ and } \deg(\phi,\Gamma_i) = d_i\}.$$

Sketch of the proof of Theorem 1. The proof is divided into two distinct parts:

Part A : The upper bound $E \leq 8\pi L$

Part B : The lower bound $E \geq 8\pi L$.

Part A: The upper bound $E \leq 8\pi L$.

The main ingredient in the proof is a basic dipole construction summarized in

Lemma 1 Consider a dipole $\{p,n\}$. Then, for every $\varepsilon > 0$ there is a map $\phi_\varepsilon \in \mathcal{E}$ (relative to the dipole), i.e.,

$$\phi_\varepsilon \in C^1(\mathbb{R}^3 \setminus \{p,n\};S^2) \text{ , } \deg(\phi_\varepsilon \text{ , } p) = +1 \text{ , } \deg(\phi_\varepsilon,n) = -1$$

such that

$$\int |\nabla\phi_\varepsilon|^2 \leq 8\pi \; |p - n| + \varepsilon \tag{5}$$

and

(6) ϕ_ε is constant outside an ε - neighborhood of the segment $[p,n]$.

Proof Without loss of generality we may assume that $p = (0,0,1)$ and $n = (0,0,-1)$. Let $\Pi: R^2 \to S^2$ be the inverse of stereographic projection from the north pole N . It is easy to check that

$$\int_{\mathbb{R}^2} |\nabla\Pi|^2 = 8\pi .$$

By a small modification of Π near infinity we obtain a smooth map $\omega_\varepsilon : \mathbb{R}^2 \to S^2$ such that

$$\begin{cases} \int|\nabla\omega_\varepsilon|^2 < 8\pi + \varepsilon \\ \omega_\varepsilon \text{ is constant } (=N) \text{ far out} \\ \deg \omega_\varepsilon = 1 \quad (\mathbb{R}^2 \cup \{\infty\} \text{ is identified with } S^2). \end{cases}$$

After a dilation we may further assume that ω_ε is constant outside the unit disc (note that $\int|\nabla\omega_\varepsilon|^2$ is invariant under dilations).

Next, consider the map $\phi : \mathbb{R}^3 \to S^2$ defined by

$$\phi(x,y,z) = \begin{cases} N & \text{if} \quad |z| > 1 \\ \omega_\varepsilon \left(\frac{x}{1-z^2}, \frac{y}{1-z^2}\right) & \text{if} \quad |z| < 1 \end{cases}$$

and the sequence of maps $\phi_n : \mathbb{R}^3 \to S^2$ defined by

$$\phi_n(x,y,z) = \phi(nx,ny,z) .$$

Note that $\phi_n \in \mathcal{E}$ and moreover ϕ_n is constant (= N) outside the region

$$V_n = \{(x,y,z) \mid z^2 + n\sqrt{x^2 + y^2} < 1 \}$$

which is a small neighborhood of the segment $[p,n]$.

We have

$$\frac{\partial\phi_n}{\partial x} = \frac{n}{1-z^2}\,\frac{\partial\omega_\varepsilon}{\partial x}\left(\frac{nx}{1-z^2}\,,\,\frac{ny}{1-z^2}\right)$$

$$\frac{\partial\phi_n}{\partial y} = \frac{n}{1-z^2}\,\frac{\partial\omega_\varepsilon}{\partial y}\left(\frac{nx}{1-z^2}\,,\,\frac{ny}{1-z^2}\right)$$

$$\frac{\partial\phi_n}{\partial z} = \frac{2nz}{(1-z^2)^2}\quad x\,\frac{\partial\omega_\varepsilon}{\partial x}\left(\frac{nx}{1-z^2}\,,\,\frac{ny}{1-z^2}\right) + y\,\frac{\partial\omega_\varepsilon}{\partial y}\left(\frac{nx}{1-z^2}\,,\,\frac{ny}{1-z^2}\right) .$$

So that

$$\frac{|\partial\phi_n|}{\partial z} < \frac{2nz}{(1-z^2)^2}\,\sqrt{x^2+y^2}\;C_\varepsilon < \frac{2z}{1-z^2}\;C_\varepsilon \qquad \text{in } V_n ,$$

where $C_\varepsilon = \operatorname{Max} |\nabla\omega_\varepsilon|$. It follows that

$$\int_{R^3} |\nabla\phi_n|^2 < 2\int_{R^2} |\nabla\omega_\varepsilon|^2 + 4\,C_\varepsilon^2 \int_{V_n} \frac{z^2}{(1-z^2)^2}\,dxdydz$$

(in order to compute the first two integrals one uses the change of variable $\zeta = \frac{nx}{1-z^2}$, $\eta = \frac{ny}{1-z^2}$) .

Therefore we obtain

$$\int_{\mathbb{R}^3} |\nabla\phi_n|^2 < 2\,(8\pi + \varepsilon) + \frac{8\pi}{3}\,C_\varepsilon^2\,\frac{1}{n^2}$$

and the conclusion follows by choosing n large enough.

In the general case, let $C = \bigcup_{i=1}^{k} [p_i , n_{\sigma(i)}]$ be any minimal connection. On each segment $[p_i, n_{\sigma(i)}]$ consider the basic dipole construction as above and then glue these objects. Note that they glue well since ϕ_ε is constant (=N) outside a small neighborhood of [p,n] and also since two segments have no self-intersection because C is a minimal connection. [Two segments may overlap or intersect at their end points but these cases are easy to handle].

Part B: The Lower Bound $E > 8\pi L$.

We have to prove that

(7) $$\int |\nabla\phi|^2 > 8\pi L \qquad \forall\ \phi \in \mathcal{E} .$$

For this purpose it is extremely convenient to associate with every map $\phi \in \mathcal{E}$ a vector field D (a kind of electric field) defined by its coordinates

(8) $$D = (\phi \cdot \phi_y \wedge \phi_z\ ,\ \phi \cdot \phi_z \wedge \phi_x\ ,\ \phi \cdot \phi_x \wedge \phi_y) .$$

The vector field D has some remarkable properties. First, we have

(9) $$|D| < \frac{1}{2} |\nabla\phi|^2 \qquad \text{on } \mathbb{R}^3 .$$

Indeed, choose a coordinate system so that

$$\phi = (0, 0, 1)$$

and then, since $|\phi| = 1$, we may write

$$\phi_x = (a_1\ , b_1\ , 0)$$
$$\phi_y = (a_2\ , b_2\ , 0)$$
$$\phi_z = (a_3\ , b_3\ , 0) .$$

Therefore we find

$$D = a \wedge b$$

with $a = (a_1, a_2, a_3)$ and $b = (b_1\ , b_2, b_3)$.

It follows that

$$|D| < |a|\ |b| < \frac{1}{2} (|a|^2 + |b|^2) = \frac{1}{2} |\nabla\phi|^2 .$$

Next, we have

(10) $$\operatorname{div} D = 4\pi \sum_{i=1}^{N} d_i \, \delta_{a_i} \qquad \text{in } \mathcal{D}'(\mathbb{R}^3) .$$

[Note that $D \in L^1$ since $\int |\nabla\phi|^2 < \infty$, and thus (10) makes sense in $\mathcal{D}'$].
Indeed, it is easy to check that

$$\operatorname{div} D = 0 \qquad \text{in } \mathbb{R}^3 \setminus \bigcup_{i=1}^{N} \{a_i\} .$$

In order to prove (10) it suffices to observe that if Σ is any smooth closed surface in $R^3 \setminus \bigcup_{i=1}^{N} \{a_i\}$, then the flux of D across Σ is given by

$$\int_{\Sigma} D \cdot \nu \, d\sigma = \int_{\Sigma} J_{\phi} \, d\sigma$$

where ν is the normal to Σ and J_ϕ is the Jacobian determinant of ϕ <u>restricted</u> to Σ ; on the other hand the degree of ϕ (considered as a map from Σ to S^2) is given by an analytic formula (see e.g. [13])

$$\deg \phi_{|\Sigma} = \frac{1}{4\pi} \int_{\Sigma} J_{\phi} \, d\sigma .$$

It is a surprising fact that we may now ignore the map ϕ and work only with the vector field D. More precisely, we claim

(11) $$\int |D| \geq 4\pi L$$

for every $D \in L^1(\mathbb{R}^3, \mathbb{R}^3)$ such that $\operatorname{div} D = 4\pi \sum_{i=1}^{N} d_i \, \delta_{a_i}$.

Note that, in view of (9) and (10), (11) implies (7). Let $\zeta : \mathbb{R}^3 \to \mathbb{R}$ be any function with $\|\zeta\|_{Lip} \leq 1$, so that $\|\nabla\zeta\|_{L^\infty} \leq 1$. We have

$$\int |D| \geq - \int D \cdot \nabla\zeta = 4\pi \sum_{i=1}^{N} d_i \, \zeta(a_i) .$$

Relabelling the points (a_i) as positive and negative points and taking into account their multiplicity we may write

$$\sum_{i=1}^{N} d_i \, \zeta(a_i) = \sum_{i=1}^{k} (\zeta(p_i) - \zeta(n_i)) .$$

Claim (11) is a consequence of the following general Lemma:

Lemma 2 Let M be a metric space and let $p_1, p_2, \dots p_k$ and $n_1, n_2, \dots n_k$ be $2k$ points in M.

Then

$$(12) \qquad \operatorname*{Max}_{\substack{\zeta : M \to \mathbb{R} \\ \|\zeta\|_{Lip} \leq 1}} \left\{ \sum_{i=1}^{k} (\zeta(p_i) - \zeta(n_i)) \right\} = L$$

where
$$\|\zeta\|_{Lip} = \operatorname*{Sup}_{x \neq y} |\zeta(x) - \zeta(y)| / d(x,y)$$

and
$$L = \operatorname*{Min}_{\sigma} \sum_{i=1}^{k} d(p_i, n_{\sigma(i)}) .$$

Proof of Lemma 2 It is clear

$$\sum (\zeta(p_i) - \zeta(n_i)) \leq \sum_{i=1}^{k} d(p_i , n_{\sigma(i)}) .$$

for every function ζ with $\|\zeta\|_{Lip} \leq 1$ and every permutation σ. It follows that

$$\operatorname*{Sup}_{\|\zeta\|_{Lip} \leq 1} \left\{ \sum (\zeta(p_i) - \zeta(n_i)) \right\} \leq L .$$

In order to prove equality it suffices to construct a function ζ defined <u>only</u> on the set $Q = \left(\bigcup_{i=1}^{k} \{p_i\} \right) \cup \left(\bigcup_{i=1}^{k} \{n_i\} \right)$ with $\|\zeta\|_{Lip} \leq 1$ on Q and such that

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

[Because such a function ζ may be extended to all of M by letting

$$\tilde{\zeta}(x) = \operatorname*{Inf}_{y \in Q} \{ \zeta(y) + d(x,y) \}$$

which has all the required properties].

The existence of ζ is a consequence of two facts:

a) A min-max equality of Kantorovich [12] (see also [14]) which - in our special situation - says that

$$\operatorname*{Max}_{\substack{\zeta:\, Q \to R \\ \|\zeta\|_{Lip} \leq 1}} \{ \sum(\zeta(p_i) - \zeta(n_i)) \} = \operatorname*{Inf}_{(a_{ij}) \in \mathcal{A}} \sum_{i,j=1}^{k} a_{ij}\, d(p_i,n_j)$$

where $\mathcal{A}$ denotes the (convex) set of doubly stochastic matrices, i.e.

$$a_{ij} \geq 0 \quad \forall\, i,j \quad , \quad \sum_{i=1}^{k} a_{ij} = 1 \quad \forall j \quad \text{and} \quad \sum_{j=1}^{k} a_{ij} = 1 \quad \forall i \quad .$$

b) A classical result of Birkhoff which asserts that the extreme points of $\mathcal{A}$ are the permutation matrices.

For the convenience of the reader we present a direct elementary argument. After relabelling the points (n_i) we may always assume that L is given by

$$L = \sum_{i=1}^{k} d(p_i,n_i) \ .$$

Set $d_i = d(p_i,n_i)$ and consider $\lambda_i = \zeta(n_i)$, $1 \leq i \leq k$, as being the unknowns so that $\zeta(p_i) = \lambda_i + d_i$. We are led to the following system of inequalities which expresses that $\|\zeta\|_{Lip} \leq 1$ on Q :

$$(13_1) \qquad | \lambda_i - \lambda_j | \leq d\,(n_i, n_j) \qquad \forall i,j$$

$$(13_2) \qquad | (\lambda_i + d_i) - (\lambda_j + d_j) | \leq d(p_i, p_j) \qquad \forall i,j$$

(13_3) $$| (\lambda_i + d_i) - \lambda_j | < d(p_i, n_j) \qquad \forall i,j \quad ,$$

which in turn is equivalent to

(14) $$\lambda_i + d_i - \lambda_j < d(p_i, n_j) \qquad \forall i,j$$

[All the other inequalities in (13) are consequences of (14) and of the triangle inequality]. In other words, we have to find a solution (λ_i) for a linear programming system of the form

(15) $$\lambda_i - \lambda_j < b_{ij} \qquad \forall i,j = 1,2,\dots k$$

where $$b_{ij} = d(p_i, n_j) - d_i \quad .$$

Such a system has a solution if and only if the matrix (b_{ij}) satisfies the condition

(16) $$\begin{cases} b_{ii} > 0 & \text{for every} \quad i = 1,2,\dots k \\ \sum_{i=1}^{k} b_{i,\sigma(i)} > 0 & \text{for every permutation} \quad \sigma \quad , \end{cases}$$

which in our case, is precisely the assumption that L is the length of a minimal connection.

Indeed, assume that (16) holds. We shall construct a solution of (15) by using essentially the method of [1]. By a chain K we mean any finite sequence of elements (not necessarily distinct) taken from $\{1,2,\dots k\}$; we write

$$K = \{n_1, n_2, \dots n_\ell\}$$

where $\ell > 2$ can be any integer. We say that a chain is a <u>loop</u> if $n_1 = n_\ell$ and we say that the chain K <u>connects</u> i to j if $n_1 = i$ and $n_\ell = j$. Given a chain K we set

$$S_K = b_{n_1 n_2} + b_{n_2 n_3} + \dots b_{n_{\ell-1} n_\ell} \quad .$$

It follows from assumption (16) that $S_K > 0$ for every loop K. This is obvious if K is a simple loop (i.e. all elements are distinct except the two end points) because we may apply (16) to the permutation $\sigma : n_1 \to n_2$, $n_2 \to n_3$, ... $n_{\ell-1} \to n_1$ with all other integers being invariant. If K is a general loop we may split it as the union of simple loops.

For every integer $i = 1, 2, \dots k$, set

$\lambda_i = \operatorname{Inf} \{ S_K \mid K$ is a chain connecting i to $1 \}$.

Note that λ_i is well defined ($\lambda_i > -\infty$) since for every chain K connecting i to 1, we have $S_K > -b_{1i}$ (because $\{1, K\}$ is a loop). It is clear that (λ_i) satisfies (15). Indeed if K is any chain connecting j to 1, then $\{i, K\}$ is a chain connecting i to 1 and so

$$\lambda_i \le b_{ij} + S_K ,$$

which implies that $\lambda_i \le b_{ij} + \lambda_j$

The proof of Theorem 2 is more delicate (see [4].) I will only give a brief indication in the case of a dipole $\{a_1, a_2\}$. First, note that if B is a ball of radius R centered at a and $\phi \in C^1(B \setminus \{a\}; S^2)$ with $\deg(\phi,a) = 1$, then,

$$\int_B |\nabla\phi|^2 \ge 8\pi R . \tag{17}$$

Indeed, consider the D field associated with ϕ.
We have

$$\int_B |\nabla\phi|^2 \ge 2 \int_B |D| \ge -2 \int_B D \cdot \nabla\zeta = 8\pi\, \zeta(0)$$

for every function ζ such that $\|\nabla\zeta\|_{L^\infty} \le 1$ and $\zeta = 0$ on ∂B; then, choose ζ to be the distance to $\partial\Omega$. Assume now, by contradiction, that the least energy E is achieved for the dipole by a map ϕ. Let B_1 (respectively B_2) be a ball centered at a_1 (respectively a_2) with radius R_1 (respectively R_2) such that $R_1 + R_2 = |a_1 - a_2| = L$. By (17) we have

$$\int_{B_1} |\nabla\phi|^2 \geq 8\pi R_1 \quad \text{and} \quad \int_{B_2} |\phi|^2 \geq 8\pi R_2$$

and thus

$$\int_{B_1 \cup B_2} |\phi|^2 \geq 8\pi(R_1 + R_2) = 8\pi L \quad .$$

Since, on the other hand,

$$\int_{R^3} |\nabla\phi|^2 = 8\pi L ,$$

we conclude that $\nabla\phi = 0$ outside $B_1 \cup B_2$. By varying R_1 and R_2 we find that $\nabla\phi = 0$ outside the segment $[a_1,a_2]$, so that ϕ is constant on R^3 - which is absurd. In fact this argument shows that if (ϕ_n) is a minimizing sequence then

$$\int_K |\nabla\phi_n|^2 \to 0$$

for every compact set K such that $K \quad [a_1,a_2] = \emptyset$. It follows that $|\nabla\phi_{n_k}|^2$ converges to a measure μ concentrated on the segment $[a_1,a_2]$. A similar argument shows that μ is uniformly distributed on the segment $[a_1,a_2]$

2. Free Singularities

Let $\Omega \quad R^3$ be a (smooth) bounded domain. Let $g: \partial\Omega \to S^2$ be a given boundary data. We consider now the problem of minimizing the energy in the class

$$= \{ \phi \in H^1(\Omega;S^2) \mid \phi = g \quad \text{on} \quad \partial\Omega \}$$

where $H^1(\Omega;S^2) = \{\phi \in H^1(\Omega; R^3) \mid |\phi| = 1 \text{ a.e. on } \Omega\}$. It is clear, by a standard lower semicontinuity argument, that

$$E = \underset{\phi \in}{\text{Min}} \int |\nabla\phi|^2$$

is achieved. Moreover, every minimizer satisfies the Euler equation i.e. the equation of harmonic maps

$$- \Delta\phi = \phi|\nabla\phi|^2 \qquad \text{on} \quad \Omega \quad .$$

[The Lagrange multiplier $|\nabla\phi|^2$ comes from the constraint $|\phi| = 1$] . It is known (see [15], [16]) that every minimizer is smooth, except at a finite number of points. In contrast with Section 1, the number and the location of the singularities is not prescribed and in fact, it would be interesting to estimate the number of singularities. Here, singularities are free to appear wherever they want as long as they help to lower the energy. A natural question is whether singularities really appear. The answer is yes and there are two reasons:

1) If $\deg(g, \partial\Omega) \neq 0$, there is a topological obstruction since g can not be extended smoothly inside Ω ; every map in the class $\mathcal{E}$ must have at least one singularity.

2) If $\deg(g, \partial\Omega) = 0$, there is no topological obstruction : g can be extended smoothly inside Ω . A very interesting example of Hardt-Lin [11] shows that there may still be singularities. In other words, the system is not forced (topologically) to have singularities, but it pays for the system to create singularities in order to lower its energy. Here is an alternative simple example of a map g from $\partial\Omega$ to S^2 , of degree zero, such that

$$E = \inf_{\substack{\phi \in H^1(\Omega;S^2) \\ \phi = g \text{ on } \partial\Omega}} \int |\nabla\phi|^2 \sim \varepsilon \tag{18}$$

while

$$E_{reg} = \inf_{\substack{\phi \in C^1(\overline{\Omega};S^2) \\ \phi = g \text{ on } \partial\Omega}} \int |\nabla\phi|^2 \sim 16\pi \tag{19}$$

(with ε arbitrarily small). Let Ω be the unit ball with north pole N and south pole S . Along the NS axis we place two dipoles with the same orientation: $\{p_1, n_1\}$ is centered at N and $\{p_2, n_2\}$ is centered at S (see Fig. 1) .

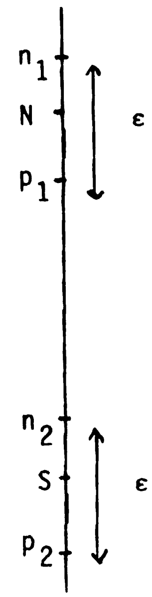

Fig. 1

We assume that $|p_1 - n_1| = |p_2 - n_2| = \varepsilon$ is small. Using the construction of Lemma 1 we obtain a map ϕ_ε which is smooth except at the points $\{p_1, n_1, p_2, n_2\}$, which is constant except on $B(N, \varepsilon/2)$ and $B(S, \varepsilon/2)$ and such that

$$\int |\nabla\phi_\varepsilon|^2 < 16\pi\varepsilon + 2\varepsilon .$$

Define g to be the restriction of ϕ_ε to $\partial\Omega$, so that g is smooth and g has degree zero. Clearly we have $E < 16\pi\varepsilon + 2\varepsilon$ (since we may use ϕ_ε as an admissible map). For the proof of (19) it is convenient to use the D field associated with ϕ; we find

$$\int_\Omega |\nabla\phi|^2 \geq 2\int_\Omega |D| \geq 2\int_\Omega D \cdot \nabla\zeta = 2\int_{\partial\Omega} (D\cdot n)\zeta \, d\sigma$$

(since $\operatorname{div} D = 0$ because ϕ is smooth), for every function ζ such that $\|\nabla\zeta\|_{L^\infty} \leq 1$. Choosing a function ζ such that $\zeta \equiv 0$ in $B(S, \varepsilon/2)$ and $\zeta \equiv 2-\varepsilon$ in $B(N, \varepsilon/2)$ we obtain

$$\int|\nabla\phi|^2 \geq 2\,(2-\varepsilon)\int_{\partial\Omega \cap B(N,\varepsilon/2)} (D \cdot n) .$$

But $D \cdot n = \operatorname{Jac} g$ is the Jacobian determinant of g, which vanishes except near N and S , and thus

$$\frac{1}{4\pi} \int_{\partial\Omega \cap B(N,\varepsilon/2)} (D \cdot n) = \deg(\phi_\varepsilon, p_i) = 1 .$$

Remark 3 This gap phenomenon $(E < E_{reg})$ raises many interesting questions:

a) Is E_{reg} achieved?

b) It implies that smooth maps from B^3 into S^2 are not dense in $H^1(B^3;S^2)$ - a fact already pointed out in [16]. More generally, one may ask whether smooth maps from B^k to S^ℓ are dense in the Sobolev space $W^{1,p}(B^k; S^\ell)$, $1 < p < \infty$. Some surprising partial results have been obtained by F. Bethuel and X. Zheng [2]. Assume for example $k = 3$:

if $\ell = 1$, smooth maps are dense iff $p \in [2,\infty)$

if $\ell = 2$ smooth maps are dense iff $p \in [1,2) \cup [3,\infty)$

if $\ell > 3$ smooth maps are dense for all $p \in [1,\infty)$.

The main results of Section 2 are the following

Theorem 3 Assume Ω is the unit ball and $g(x) = x$ is the identity map on $\partial\Omega$. Then $\phi(x) = x/|x|$ is a minimizer for E .

Theorem 4 Assume Ω is the unit ball and $g : \partial\Omega \to S^2$ is arbitrary. Then the homogeneous extension $\phi(x) = g(x/|x|)$ is <u>not</u> a minimizer for E unless g is an isometry or a constant.

Remark 4 By contrast, if we ask the question whether $\phi(x) = g\,(x/|x|)$ is a critical point, i.e. a solution of $-\Delta\phi = \phi|\nabla\phi|^2$, then there are many more g's (all harmonic maps from S^2 to S^2) .

These results have an interesting consequence:

Corollary 5 Assume Ω is any domain and g is any map. Let ϕ be a minimizer for E, then all its singularities have degree ± 1. Moreover, for every singularity x_0, there is a rotation R such that

$$\phi(x) \sim \pm R\left(\frac{x - x_0}{|x-x_0|}\right) \quad \text{as} \quad x \to x_0 \ .$$

Corollary 5 is derived from Theorem 4 by a standard blow-up procedure. Assume for example $x_0 = 0$; as $\varepsilon \to 0$, $\phi(\varepsilon x) \to \psi(x)$ (see [15] and [17]) which is a minimizing harmonic map and which depends only on the direction $x/|x|$. It follows from Theorem 4 that $\psi(x) = \pm Rx / |x|$.

Sketch of the Proof of Theorem 3 Our proof is rather indirect and it would be interesting to find a different argument. An obvious calculation shows that the energy of $x/|x|$ is 8π. Therefore, we have only to prove that

(20) $$\int |\nabla\phi|^2 \geq 8\pi \qquad \forall \phi \in H^1(\Omega;S^2) \ , \ \phi(x) = x \ \text{on} \ \partial\Omega \ .$$

It suffices to establish (20) for ϕ's which are smooth except at a finite number of points. The reason is that, by [15], every minimizer has that property; alternatively one may also invoke a result of [2] which asserts that such ϕ's are dense in H^1. Consider such a ϕ and its D field. We have

$$\int_\Omega |\nabla\phi|^2 \geq 2 \int_\Omega |D| \geq 2 \int_\Omega D \cdot \nabla\zeta = 2 \int_{\partial\Omega} (D \cdot n)\zeta - 2 \int_\Omega (\operatorname{div} D)\zeta$$

for every ζ such that $\|\nabla\zeta\|_{L^\infty} \leq 1$.

But $D \cdot n = \operatorname{Jac}(\phi|_{\partial\Omega}) = 1$ (since $\phi(x) = x$ on $\partial\Omega$) and $\operatorname{div} D = \sum_{i=1}^{N} d_i \, \delta_{a_i}$ with $d_i \in \mathbb{Z}$ and $\sum_{i=1}^{N} d_i = 1$.

Therefore, we have

$$\frac{1}{8\pi} \int_\Omega |\nabla\phi|^2 \geq \frac{1}{4\pi} \int_{\partial\Omega} \zeta \, d\sigma - \sum_{i=1}^{N} d_i \ \zeta(a_i) \ .$$

Lemma 3 below (applied with $M = \Omega$ and $d\mu = \frac{1}{4\pi} d\sigma$) shows that

$$\frac{1}{8\pi} \int_\Omega |\nabla\phi|^2 \geq \operatorname*{Min}_{y \in \overline{\Omega}} \frac{1}{4\pi} \int_{\partial\Omega} |y-\sigma| d\sigma = 1 .$$

Lemma 3 Let M be a compact metric space and let μ be a fixed probability measure on M .

Then

$$\operatorname*{Inf}_{\nu \in \mathcal{A}} \operatorname*{Max}_{\substack{\zeta : M \to \mathbb{R} \\ \|\zeta\|_{Lip} \leq 1}} \{ \int \zeta d\mu - \int \zeta d\nu \} = \operatorname*{Min}_{y \in M} \int d(x,y) d\mu(x)$$

where the infimum is taken over the class $\mathcal{A}$ of all measures ν of the form $\nu = \sum_{\text{finite}} d_i \, \delta_{a_i}$, with $d_i \in \mathbb{Z}$ and $\sum d_i = 1$.

Sketch of the Proof of Lemma 3 It is clear that $\operatorname*{Inf}_{\nu} \operatorname*{Max}_{\zeta} \leq \operatorname*{Min}_{y}$. Indeed, if we choose $\nu = \delta_y$ we obtain

$$\int \zeta d\mu - \int \zeta d\nu = \int (\zeta(x) - \zeta(y)) d\mu(x) \leq \int d(x,y) d\mu(x) .$$

For the reverse inequality, it suffices - by density - to consider the case where μ is a discrete measure with rational coefficients, which we may always write as

$$\mu = \frac{1}{m} \sum_{i=1}^{m} \delta_{c_i}$$

(the points c_i need not be distinct).

Fix a measure $\nu \in \mathcal{A}$; relabelling the points (a_i) as positive and negative points and taking into account their multiplicity we may write

$$\nu = \sum_{j=1}^{k} \delta_{p_j} - \sum_{j=1}^{k-1} \delta_{n_j} .$$

We have to prove that $A \geq B$ where

$$A = \max_{\|\nabla\zeta\|_{Lip} \leq 1} \left\{ \int \left(m \sum_{j=1}^{k} \delta_{p_j} - m \sum_{j=1}^{k-1} \delta_{n_j} - \sum_{i=1}^{m} \delta_{c_i}\right)\zeta \right\}$$

and

$$B = \min_{y \in M} \sum_{i=1}^{m} d(c_i, y) .$$

It follows from Lemma 2 that $A = L$, the length of a minimal connection of a system which consists of mk positive points and mk negative points. The positive points are the points $(p_j)_{1 \leq j \leq k}$ counted with multiplicity m. The negative points are the points $(n_j)_{1 \leq j \leq k-1}$ counted with multiplicity m together with the points $(c_i)_{1 \leq i \leq m}$ counted with multiplicity one. Finally we invoke the following Lemma from Graph Theory (whose statement has been conjectured by us and proved by Hamidoune-Las Vergnas [9])

Lemma 4 Consider a family of k boys $B_1, B_2 \ldots B_k$ and k girls $G_1, G_2 \ldots G_k$. Assume $\mathcal{G}$ is a graph connecting the boys and the girls such that, in $\mathcal{G}$, every boy is joined exactly to m girls and every girl is joined exactly to m boys. Then, given any girl G there is some boy B joined to G by m disjoint paths in $\mathcal{G}$.

Proof of Lemma 3 completed

The boys are the points $p_1, p_2, \ldots p_k$; the girls $G_1, G_2, \ldots G_{k-1}$ are the points $n_1, n_2, \ldots n_{k-1}$, while G_k consists of $\bigcup_{i=1}^{m} \{c_i\}$. The graph $\mathcal{G}$ is any minimal connection.

It follows from Lemma 4, that given the girl $G = G_k$, there is some boy, say p_ℓ, such that $\mathcal{G}$ contains m disjoint paths joining p_ℓ to all the points $(c_i)_{1 \leq i \leq m}$. We conclude that

$$L \geq \sum_{i=1}^{m} d(c_i, p_\ell) \geq \min_{y \in M} \sum_{i=1}^{m} d(c_i, y) = B .$$

The proof of Theorem 4 is quite involved and I will not discuss it here (see [3]). Rougly speaking, there are two steps:

Step 1 If $|\deg g| > 1$ one constructs a map ϕ with more than one singularity and with energy lower than $g(x/|x|)$

Step 2 If $|\deg g| = 1$ and g is not an isometry, one can lower the energy by "moving the singularity" towards the center of mass of $|\nabla g|^2$ i.e. $\int_{\partial\Omega} |\nabla g|^2 \sigma d\sigma$.

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