

A MATHEMATICAL PROBLEM RELATED TO THE PHYSICAL THEORY OF LIQUID CRYSTAL CONFIGURATIONS

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1. INTRODUCTION

The purpose of this note is to explain a mathematical problem in liquid crystal configuration and the mathematical tools that one is naturally lead to use in order to understand it.

It will turn out that one necessarily has to understand the structure of the set of singularities of functions of bounded variation. This was first studied by the fundamental work of De-Giorgi [16], [3] and H. Federer [7]. (see also Vol'pert [15], and Simon [12]). In this note we shall explain a different method that we have used in order to study this basic fact and which is useful to study the liquid crystal problem which we shall explain in Section 2. As a matter of fact we have recovered the well known results mentioned above and furthermore we have obtained new information that we shall be briefly discussing.

Our approach is motivated by the original work of De-Giorgi on the study of the set of singularities of a characteristic function of a set of finite perimeter, see [16] p.3-62 (see also Example (B) in Section 3.2). Roughly speaking we can say that we recover

De-Giorgi's original argument and thereby we unified the theory on the structure of the set of singularities for characteristic functions of sets of finite perimeter and general bounded variation functions.

One advantage of our approach is that it gives information on sets which are not necessarily rectifiable, like rank properties of Hessian measures, see Theorem A. This information is indeed essential to show the rectifiability of relevant sets, for instance the set of points where a function of bounded variation has jump discontinuities. Together with measure theoretical arguments, see Section 3.3, this implies the decomposition. Let $u: \Omega \subseteq \mathbb{R}^n \rightarrow \mathbb{R}$

be a function of bounded variation, that is $u \in L^1(\Omega)$, Du (derivative in the distribution sense) is a finite Radon - measure. Then as measure

$$Du = Du \llcorner S \cup Du \llcorner \Omega \setminus S$$

where

- (i) $Du \llcorner \Omega \setminus S$ is absolutely continuous with respect to the Lebesgue measure on \mathbb{R}^n and the Lebesgue measure of S is zero. Here $Du \llcorner S$ is the measure defined by $(Du \llcorner S)(A) = (Du)(A \cap S)$ for every Borel set in \mathbb{R}^n ;
- (ii) S can be decomposed in $S = E \cup N$ where
 - (a) E is the set of jump discontinuity of u , that is $E = \{x \in \Omega: \limsup_x u > \liminf_x u\}$

where

$$\operatorname{ap} \limsup_x u = \sup\{\beta: \limsup_{r>0} \int_{B_r(x)} X_\beta(y) dy / r^n > 0\}$$

where $X_\beta = \chi_{F_\beta}$, $F_\beta = \{x \in \Omega: u(x) \geq \beta\}$ is the

characteristic function of the set F_β . Similarly

$$\operatorname{ap} \liminf_x u = \inf\{\beta: \limsup_{r \rightarrow 0} \int_{B_r(x)} (1 - X_\beta)(y) dy / r^n > 0\}$$

where $B_r(x)$ is the open ball of radius r with center at x .
Moreover, E is $(n-1)$ rectifiable, that is

$$E = \bigcup_{j=1}^{\infty} \Gamma_j \cup N_0 \quad (\text{disjoint union})$$

where Γ_j are compact sets contained in C^1 hypersurfaces and $H_{n-1}(N_0) = 0$ where H_{n-1} denotes the $(n-1)$ -dimensional Hausdorff measure.

(b) In the set \mathcal{L} , u is approximately continuous, that is

$$\operatorname{ap} \limsup_x u = \operatorname{ap} \liminf_x u$$

and if $H_{n-1}(A) < \infty$ then $\int_A |Du| = 0$.

(c) N is a set of zero $(n-1)$ -dimensional Hausdorff measure.

Current work suggests that our approach also gives important insight to relax the functional

$$u \rightarrow \int_{\Omega} f(u, \nabla u) dx$$

for $u \in BV(\mathbb{R}^n, \mathbb{R}^m)$ where $f(v, p): \mathbb{R}^m \times \mathbb{R}^{nm} \rightarrow \mathbb{R}$ and

(i) f is continuous in v , f is convex in p ,

(ii) $\lim_{t \rightarrow \infty} \frac{f(v, tp)}{t} = f_{\infty}(v, p)$ exists

and it is bounded uniformly in v .

If f is independent of v , $f(\nabla u)$ is defined as a measure which is lower semicontinuous with respect to the weak star topology of measures and which can be approximated by smooth functions.

However, if f depends on v the explicit definition of $f(u, \nabla u)$ for $u \in BV$ is not in the literature except for the scalar case ($m = 1$) [5] or for special choice of f when $n = 1$, see [14].

We here suggest one definition at least when f is positive and homogeneous of degree one in p ,

$$f(u, \nabla u)(A) = \int_{E \cap A} \text{dist}_f(u_+, u_-) dH_{n-1} + f(u(x), h(x)) |\nabla u| L(\Omega \setminus S)(A)$$

$E \cap A$

with

$$\text{dist}_f(u_+, u_-) = \inf_{\begin{subarray}{c} \gamma(0) = u_+ \\ \gamma(1) = u_- \end{subarray}} \int_0^1 f(\gamma(t), \dot{\gamma}(t)) dt$$

where u_+, u_- are the trace of u on E from each side, $h(x)$ is the Radon-Nikodym derivative of ∇u with respect to $|\nabla u|$, A is a Borel set in Ω and γ is a C^1 curve that joins u_+ with u_- . So far we have only checked that $f(u, \nabla u)$ is lower semicontinuous when u is piecewise constant.

In a suitable form this relaxation problem is important in the liquid crystal problem which is explained in the next section.

(2) THE LIQUID CRYSTAL PROBLEM, THE SMECTIC STATE.

In the theory of liquid crystal one has a domain Ω in R^3 , the region occupied by the liquid crystal and a unit vector field $u: \Omega \rightarrow S^2$, called the optic axis. The alignment of this axis may be influenced by external magnetic or electric fields. In any case, there is associated a free energy density due to Ossen - Frank,

$$W(\nabla u, u) = k_1(\text{div } u)^2 + k_2 (u \cdot \text{curl } u)^2 + k_3 |u \times \text{curl } u|^2 \\ + (k_2 + k_4) (\text{tr } (\nabla u)^2 - (\text{div } u)^2)$$

where the k_i are constants with $k_1, k_2, k_3 > 0$. One is interested in infima of the corresponding integral functional subject to appropriate boundary conditions.

In the special case $k_1 = k_2 = k_3$ and $k_4 = 0$, $W(\nabla u, u)$ reduces to $|\nabla u|^2$ and critical points are harmonic maps from Ω to S^2 . For energy minimizing harmonic maps from Ω to S^2 the singularities are at most isolated (Schoen-Uhlenbeck [10]) and there is good information on the asymptotic behavior near a singularity (L. Simon [13], Brezis-Coron-Lieb [2])

For the general W , Hardt-Kinderlehrer-Lin [9] shows that singularities of the solutions have Hausdorff dimension less than one. Moreover, Brezis-Coron-Lieb [2] found restrictions on limit configurations of such singularities. In liquid crystal this state is known as nematic.

In any case, in the smectic state of liquid crystal one consider solutions of the form $u = \frac{\nabla \psi}{|\nabla \psi|}$ for some function $\psi : \Omega \rightarrow \mathbb{R}$

and the level surfaces of ψ form a system of parallel surfaces

Experimentally, [11], one observes one dimensional singularities and the singularities lying in surfaces, which cannot be explained by the above theory (above, the singularities of the solution have Hausdorff dimension less than one). Simple examples and physical considerations (Ericksen [17] and Sethna [18]) suggest that the solution of the following relaxation problem explain with accuracy the phenomena.

We study the energy functional

$$G(u) = \int_{\Omega} [(|\nabla u| - 1)^2 + \varepsilon (\Delta u)^2] dx$$

where Ω is now a domain in \mathbb{R}^n , $n \geq 2$.

It is clear that if u minimizes G , then u also minimizes

$J(u) = \varepsilon^{-1/2} G(u)$. We now consider the problem

$$\text{Min } J_{\varepsilon}(u) = J_{\varepsilon}(u_{\varepsilon})$$

$$u \in H^2(\Omega) \quad u|_{\partial\Omega} = g \quad \text{or} \quad \frac{\partial u}{\partial n}|_{\partial\Omega} = 0.$$

It is a simple exercise to show that the minimum is achieved.

Heuristically we expect

$$u_{\varepsilon} \rightarrow u_0 \text{ in } H^1(\Omega)$$

$$(u_{\varepsilon})_{ij} \rightarrow (u_0)_{ij} \quad 1 \leq i, j \leq n, \text{ weakly as measures, and}$$

$$|\nabla u_0| = 1, \text{ a.e. in } \Omega, (u_0)_{ij}, \quad 1 \leq i, j \leq n \text{ are finite Radon}$$

measures. When $n = 3$ u_0 will describe the phenomena of the smectic state of liquid crystal.

We notice at once that we can use the theory described in the introduction to study the structure of the set of singularities of ∇u_0 . For instance we can use it to study the following important question: What is the limiting energy? Is this energy lower semi-continuous in the corresponding space?

To understand this question in more details we first observe that

$$J_\varepsilon(u) \geq \int_\Omega 2(|\nabla u| - 1) |\Delta u| \, dx = E_0(u)$$

It is therefore natural to conjecture that a suitable form of the energy E_0 will be the limiting energy. To formalize this, we first have to give meaning to $E_0(u)$ when $|\nabla u| = 1$ a.e. in Ω , and u_{ij} , $1 \leq i, j \leq n$, are finite Radon measures. Briefly this goes as follows. By the Radon Nikodym theorem the singular part of the measure $[D^2u]$, the modulus of the largest eigenvalue of the symmetric matrix $[u_{ij}]$, has support in

$$\Sigma = \left\{ x \in \Omega : \lim_{r \rightarrow 0} \frac{[D^2u](B_r(x))}{r^n} = \infty \right\}$$

and we may also assume that

$$\lim_{r \rightarrow 0} \frac{u_{ij}(B_r(x))}{[D^2u](B_r(x))} = A_{ij}(x), \quad \lim_{r \rightarrow 0} \frac{|u_{ij}|(B_r(x))}{[D^2u](B_r(x))} = |A_{ij}(x)|$$

exist. Theorem A, Example A in Section 3.2 and the measure theoretical relations of Section 3.3 show that (A_{ij}) has rank 1 on the set

$$S = \left\{ x \in \Sigma : \infty > \limsup_{r \rightarrow 0} \frac{[D^2u]}{r^{n-1}} > 0 \right\}$$

and $S = \bigcup_{j=1}^{\infty} \Gamma_j \cup N_0$ (disjoint union) where Γ_j are compact sets

which are contained in C^1 hypersurfaces C_j and $H_{n-1}(N_0) = 0$.

The normal to C_j on Γ_j is the eigenvector of A_{ij} , it turns out. The proposal definition of E_0 is

$$\frac{1}{2} E_0(u) = \sum_{\ell=1}^{\infty} \int_{\Gamma_{\ell}} \int \frac{\partial u}{\partial n^+} \left| \frac{\partial u}{\partial n^-} \right| \sqrt{\tau^2 + u^2} \frac{-1}{\tan} \left| d\tau \, dH_{n-1} \right.$$

for $\nabla u \in BV(\Omega)$ and $|\nabla u| = 1$ a.e. in Ω . Here $\frac{\partial u}{\partial n^-} < \frac{\partial u}{\partial n^+}$ are the trace of ∇u on the normal direction of C_j and u_{\tan} denotes trace of ∇u in the tangential directions of C_j .

So far, we have only checked this definition is compatible with important cases. The studies mentioned in the introduction suggest that $E_0(u)$ is lower-semicontinuous in $\mathcal{M} = \{u: \Omega \rightarrow \mathbb{R}, u_{ij}, 1 \leq i, j \leq n \text{ are finite Radon measures}\}$ and $u^k \rightarrow u, u^k, u \in \mathcal{M}$ if $\nabla u^k \rightarrow \nabla u$ in $L^1(\Omega)$.

To show that $J_{\varepsilon} \rightarrow E_0$ the more natural thing to try is to prove that J_{ε} converges to E_0 in the Γ -sense of De-Giorgi ([4], [14]). To verify this, assuming that E_0 is lower semicontinuous in \mathcal{M} , it suffices to show that for $u \in \mathcal{M}$, there exists u^{ε} in $H^2(\Omega)$, $u^{\varepsilon} \rightarrow u$ in \mathcal{M} and $J_{\varepsilon}(u^{\varepsilon}) \rightarrow E_0(u)$ as $\varepsilon \rightarrow 0$. We believe that this is indeed true.

3. SINGULARITIES OF FUNCTION OF BOUNDED VARIATION AND RANK PROPERTIES OF HESSIAN MEASURES.

In this section we summarize the results that it will appear in [1].

3.1. Rank properties of Hessian Measures.

We work in the following setting. Let u be a function defined in an open set $\Omega \subseteq \mathbb{R}^n$, $n \geq 1$, whose second derivatives u_{ij} , $1 \leq i, j \leq n$ are finite Radon - measures in Ω . We are interested in the singular part of u_{ij} . Let

$$\Sigma = \{x \in \Omega: \lim_{r \rightarrow 0} \frac{[D^2u](B_r(x))}{r^n} = \infty\}$$

where $[D^2u]$ is the modulus of the largest eigenvalue of the symmetric matrix $D^2u = (u_{ij})$. By the Radon-Nikodym theorem, the singular part of D^2u agrees with $D^2u \llcorner \Sigma$. We may also assume (by taking off a set of D^2u measure zero if necessary) that $x \in \Sigma$

$$\lim_{r \rightarrow 0} \frac{u_{ij}(B_r(x))}{[D^2u](B_r(x))} = A_{ij}(x) \text{ exists}$$

and

$$\lim_{r \rightarrow 0} \frac{|u_{ij}|(B_r(x))}{[D^2u](B_r(x))} = |A_{ij}(x)| \text{ exists}$$

Let now the upper density function be defined by

$$\theta_q^*(x) = \limsup_{r \rightarrow 0} \frac{[D^2u](B_r(x))}{r^q}, \quad n-1 \leq q < n.$$

Theorem A. Let

$$S_q = \{x \in \Sigma : \infty > \theta_q^*(x) > 0\} \quad n-1 \leq q < n.$$

Then on S_q , (A_{ij}) has rank one.

Note: Examples show that in general S_q is not rectifiable.

3.2. Blowing up and Rectifiability, two examples.

In this section we very briefly indicate that Theorem A, together with a blowing up argument and the Whitney criterium for rectifiability, [16] p.53, can be used to show the rectifiability of two important sets.

Example A. Let $u: \Omega \subseteq \mathbb{R}^n \rightarrow \mathbb{R}$ be a function such that:

- (i) $H(\nabla u(x)) = 1$ a . e. in Ω where $H: \mathbb{R}^n \rightarrow \mathbb{R}$ is a convex function;
- (ii) D^2u is a symmetric matrix of finite Radon measures.

Define the lower $(n-1)$ density by

$$\theta_*(x) = \liminf_{r \rightarrow 0} \frac{[D^2u](B_r(x))}{r^{n-1}}$$

Then $\mathcal{R}_1 = \{x \in \Sigma: \infty > \theta_*(x) > 0\}$ is rectifiable. Moreover, the normal vector for $x \in \mathcal{R}_1$ is given by the eigenvector of the matrix $D^2u(x) = (A_{ij}(x))$ in Theorem A.

Example B. Let A be a set of finite perimeter, that is the gradient (in the generalized sense) of the characteristic function of the set A , ∇X_A , is a finite Radon measure, that is $|\nabla X_A|(\Omega) < \infty$. Let

$$\Sigma = \{x \in \Omega: \lim_{r \rightarrow 0} \frac{|\nabla X_A|(B_r(x))}{r^n} = \infty, \\ \lim_{r \rightarrow 0} \frac{\nabla X_A(B_r(x))}{|\nabla X_A|(B_r(x))} \text{ exists}\}$$

and

$$\theta_*(x) = \lim_{r \rightarrow 0} \inf \frac{|\nabla X_A|(B_r(x))}{r^{n-1}}.$$

Then the set $\mathcal{R}_2 = \{x \in \Sigma: \infty > \theta_*(x) > 0\}$ is rectifiable

In both examples the key idea of the proof is to use the rescaled measures:

$$u_{ij}^t(K) = u_{ij}(x + tK) t^{1-n}, \quad x \in \mathcal{R}_1$$

(in Example A) or

$$(\nabla X_A)^t(K) = \nabla X_A(x + tK) t^{1-n}, \quad x \in \mathcal{R}_2$$

(in Example B) where K is an open set together with the Whitney criterium for rectifiability.

3.3 Relation Among several sets of singularities

In this section we indicate that the results used in Section 2 and De-Giorgi's decomposition of a set of finite perimeter [16] p.3-62, follow from the results in Section 3.2 and the theorem below. Also, the decomposition of a general function of bounded variation (see introduction) follows from Theorem A, a blowing up argument (similar to the one explained in Section 3.2 with the rescaled measures), the Whitney criterium for rectifiability and the theorem below. Details of the proof can be found in [1].

Let $u: \Omega \rightarrow \mathbb{R}$ be a function of bounded variation. By the Radon - Nikodym theorem, we may assume that

$$(3.1) \quad \lim_{r \rightarrow 0} \frac{Du(B_r(x))}{|Du|(B_r(x))} = n(x) \text{ exists and } |n(x)| = 1$$

(We take off a set of $|Du|$ measure zero, if necessary)

We recall for x that satisfies (3.1)

$$(i) \quad \theta^*(x) = \limsup_{r \rightarrow 0} \frac{|Du|(B_r(x))}{r^{n-1}}$$

$$(ii) \quad \theta_*(x) = \liminf_{r \rightarrow 0} \frac{|Du|(B_r(x))}{r^{n-1}}$$

(iii) x is a Lebesgue point of u if there exists c such that

$$\lim_{r \rightarrow 0} \frac{1}{|(B_r(x))|} \int_{B_r(x)} |u(y) - c| dy = 0$$

We denote the set of Lebesgue points of u by \mathcal{L} . By E we denote the set of jump discontinuities (see introduction). Then we have the following result.

THEOREM B (a) If $x \in \mathcal{L}$, then $\theta^*(x) = 0$

(b) If $x \in E$, then $\theta^*(x) > 0$.

(c) \mathcal{H}_{n-1} a.e. $x \in E$, $\theta_*(x) > 0$. Furthermore \mathcal{H}_{n-1} a.e. $x \in E$
 $\theta_*(x) = \theta^*(x)$.

(d) \mathcal{H}_{n-1} a.e. if $x \notin E$, then $x \in \mathcal{L}$.

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