Singular Minimizers and their Significance in Elasticity

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1. INTRODUCTION.

Minimizers of integrals of the calculus of variations typically possess singularities. For problems arising from mechanics, such singularities may represent physically interesting instabilities. We explore this here in the context of elasticity theory, for which a complete classification of possible singularities is not known. Certainly, as will be described below, singular minimizers exist that model aspects of solid phase transformations and certain modes of fracture. But it remains to be seen if certain singularities encountered elsewhere in the calculus of variations can occur in elasticity, or whether these are eliminated as a consequence of low spatial dimensions and invariance requirements. Perhaps some such singularities are already in the experimental literature for those with the eyes to see them.

The plan of the paper is as follows. In §2 the basic problem of energy minimization in elasticity is described, together with a bare minimum of information concerning properties of the stored-energy function. In each of the subsequent sections a particular type of singularity is discussed, the order being roughly that of increasing degree of singularity.

DIRECTIONS IN PARTIAL
DIFFERENTIAL EQUATIONS

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indifference condition

$$W(x,QA) = W(x,A) \quad \text{for all} \quad Q \in SO(n), \tag{2.3}$$

which asserts that the elastic energy of a body is unaffected by a rigid rotation. In addition W may satisfy material symmetries, such as the isotropy condition

$$W(x,AQ) = W(x,A) \quad \text{for all} \quad Q \in SO(n). \tag{2.4}$$

It is well known (see [6] for a discussion and the classical references) that (2.3),(2.4) together imply that

$$W(x,A) = \Phi(x; v_1,\ldots,v_n), \tag{2.5}$$

for some function Φ that is invariant to permutations of the eigenvalues $v_i = v_i(A)$, $1 \leqslant i \leqslant n$, of $\sqrt{A^TA}$. These eigenvalues are usually called the principal stretches. Elastic crystals are not in general isotropic, but satisfy more complicated symmetry conditions related to their lattice structure.

In order to set up the minimization problem more precisely it is necessary to introduce a function space of admissible deformations. The choice of this function space involves in particular a choice for the meaning to be attached to Du, for a nonsmooth deformation u, which can dramatically affect the predictions of the model. The rationale for preferring one function space to another warrants further study. In this paper we consider the problem of minimizing I in the set

$$\mathcal{A}_p = \{u \in W^{1,p} : u|_{\partial\Omega_1} = f\}.$$

Here and below, for $1 \leqslant p \leqslant \infty$, $W^{1,p} = W^{1,p}(\Omega;\mathbb{R}^n)$ denotes the usual Sobolev space of mappings $u : \Omega \to \mathbb{R}^n$.

Note that minimizers u of I in $\mathcal{A}_p$ formally satisfy on $\partial\Omega \setminus \partial\Omega_1$ the natural boundary condition

$$\frac{\partial W}{\partial A}(x,DU)\ N(x) = 0, \tag{2.6}$$

where $N(x)$ denotes the unit outward normal to $\partial\Omega$ at x. This expresses the fact that the surface traction on $\partial\Omega$ at x is zero.

(b) smooth non-affine minimizers

For realistic models of elastic materials with W smooth no examples of absolute minimizers of I in $\mathcal{A}_p$, or even of 'strong relative minimizers' (cf Ball & Marsden [11]), that are smooth but not affine are known to the author. (The example described in §4 below could perhaps be thought of as of this type, but the properties of the stored-energy function necessary for the example have not been correlated with those of any real material, and the stress distribution is in any case trivial.) Although such smooth minimizers presumably abound their existence is hard to establish for two reasons. First, although the existence of nontrivial absolute minimizers can be proved via the direct method of the calculus of variations, no regularity theory for minimizers is available even under the mathematically most favourable realistic hypotheses; the most that is known is the partial regularity theorem of Evans [23] (see also Evans & Gariepy [24]), which still needs improvement to accommodate singular behaviour of $W(A)$ as $\det A \to 0+$. Second, although smooth non-affine solutions of the equilibrium equations (i.e. the Euler-Lagrange equations for (3.1)) are known, no extension of the field theory of the calculus of variations to dimensions $n > 1$ is available that might apply to elasticity (see Morrey [39 p15], Ball & Marsden [11]) and enable one to show that a particular solution is a minimizer.

4. MINIMIZERS SINGULAR ONLY ON THE BOUNDARY.

The work in the section is taken from Ball & James [9]. We consider a stored-energy function of a type analyzed in [5 §6.4] and Ball & Marsden [11]. To construct it let $1 < \alpha < n$, $0 < \lambda < \mu < \infty$ and let $\phi : (0,\infty) \to (0,\infty)$ satisfy (i) ϕ is smooth, (ii) $\phi' > 0$, $\phi'' > 0$, and (iii) $\phi(v) = v^\alpha$ for $\lambda \leq v \leq \mu$. Now choose $h : (0,\infty) \to \mathbb{R}$ satisfying (i) h is smooth, (ii) $h'' > 0$, (iii) $h(\tau) = -n\tau^{\alpha/n}$ for $\lambda^n \leq \tau \leq \mu^n$, and (iv) $h(\tau) > -n\phi(\tau^{1/n})$ for $\tau \notin [\lambda^n, \mu^n]$. Such functions h exist because $(\tau^{\alpha/n})'' < 0$ for $\lambda^n \leq \tau \leq \mu^n$.

Define

$$\Phi(v_1,\ldots,v_n) = \sum_{i=1}^{n} \phi(v_i) + h\Big(\prod_{i=1}^{n} v_i\Big), \tag{4.1}$$

study of regularity up to the boundary of linear elliptic systems.

Turning to the case $n \geqslant 3$, the conformal transformations are now characterized by Liouville's theorem as products of inversions. Under our regularity assumptions (i.e. $u \in W^{1,\infty}$, using (4.4)) an appropriate version of Liouville's theorem has been proved by Reshetnyak [42]. For n odd an example is given by

$$u(x) = -\frac{x}{|x|^2}. \tag{4.5}$$

If $0 \notin \bar{\Omega}$ then u satisfies (4.4) with $v(x) = |x|^{-2}$. Note that when Ω is convex this furnishes an example of a non-trivial deformation which is an absolute minimizer of the energy for a strictly polyconvex isotropic material with zero traction boundary conditions, and thus bears on a conjecture of Noll [41] (see also Truesdell [50]) to the effect that for rubber-like materials the absolute minimizer is homogeneous and unique up to rigid-body translation and rotation.

5. LIPSCHITZ MINIMIZERS.

The work in this section is also taken from Ball & James [9]. We are interested here in minimizers $u \in W^{1,\infty}$ (i.e. u Lipschitz) which are not smooth in Ω. The simplest such minimizers are piecewise affine. A piecewise affine deformation u is one for which

$$Du(x) \in \{A_1,\ldots,A_M\} \quad \text{a.e. } x \in \Omega,$$

with meas $S_i > 0$ for $i = 1,\ldots,M$, where

$$S_i = \{x \in \Omega: Du(x) = A_i\},$$

$M \geqslant 2$ and the $A_i \in M_+^{n\times n}$ are distinct. Deformations of elastic crystals that are to a good approximation piecewise affine are commonly observed. The matrices A_i in a piecewise affine deformation are not arbitrary, and in this direction we record without proof two results. First, if $M = 2$ then necessarily

$$A_2 - A_1 = \lambda \otimes \mu \tag{5.1}$$

for some $\lambda, \mu \in \mathbb{R}^n$. This is a generalization of the jump to b and of width $1/j$, and such that

$$\lim_{j\to\infty} I(u^{(j)}) = \int_{\Omega\cap\{x^3<0\}} W(x^3,A_3)\,dx + \int_{\Omega\cap\{x^3>0\}} W(x^3,A_1)\,dx. \quad (5.3)$$

Hence $\inf_{\mathcal{A}_p} I$ is given by the right-hand side of (5.3), and such sequences $u^{(j)}$ are minimizing. The finely layered deformations in these minimizing sequences are similar to those observed, for example, by Saburi & Wayman [43] in shape memory martensites and by Burkart & Read [15] for indium-thallium twins. They are also reminiscent of layering in the theory of optimal design of composite materials (cf Francfort & Murat [25], Kohn & Strang [34], Lurie & Cherkaev [35], Milton [37]). We claim that the absolute minimum of I in $\mathcal{A}_p$ is not attained. If it were then any minimizer u would satisfy in a neighbourhood of the origin

$$u(x) = \begin{cases} u(0) + x + \lambda(b\cdot x)a & \text{for } x^3 > 0 \\ u(0) + x + x^3 c & \text{for } x^3 < 0, \end{cases} \quad (5.4)$$

where $\lambda \in W^{1,\infty}(\mathbb{R})$ with $\lambda(0) = 0$ and $\lambda'(t) = \pm 1$ a.e.. Applying the continuity of u on $x^3 = 0$ gives a contradiction.

6. CONTINUOUS MINIMIZERS WITH UNBOUNDED DERIVATIVES.

It is not known whether continuous minimizers u with Du unbounded can occur for realistic models of elastic materials. If such minimizers exist, they would be of importance as a mechanism for the initiation of fracture or dislocations. The existence of such singular minimizers is suggested by the one-dimensional examples of Ball & Mizel [12,13] of regular (i.e. elliptic) integrals whose minimizers among appropriate classes of absolutely continuous functions have unbounded derivatives, and do not satisfy the usual weak form of the Euler-Lagrange equation. One of these examples is the integral

$$I(u) = \int_{-1}^{1} [(u^6 - x^4)^2 |u'|^s + \varepsilon(u')^2]\,dx, \quad (6.1)$$

where $s > 27$ and $\varepsilon > 0$ is sufficiently small. The absolute minimum of I in $\mathcal{A} = \{u \in W^{1,1}(-1,1): u(-1) = -1, u(1) = 1\}$ is attained, and every minimizer u_0 satisfies quasiconvex at every $A \in M_+^{3\times3}$ if and only if $3 \leqslant p \leqslant \infty$. For $1 \leqslant p < 3$ the situation is different, as can be shown by considering radial deformations, that is deformations of the form

$$u(x) = \frac{r(R)}{R} x , \tag{7.2}$$

where $R = |x|$ and $r: [0,1] \to [0,\infty)$ is increasing. Denoting by $\mathcal{A}_p^{rad}$ the set of such radial deformations in $\mathcal{A}_p$, it can be shown [5] that there exists a number $\lambda_{cr} > 0$ such that if $0 < \lambda \leqslant \lambda_{cr}$ then $u(x) \equiv \lambda x$ is the unique absolute minimizer of I in $\mathcal{A}_p^{rad}$ for $1 \leqslant p \leqslant \infty$, but that if $\lambda > \lambda_{cr}$ then there exists a function $r_\lambda(\cdot)$ with $r_\lambda(0) > 0$ such that the corresponding u given by (7.2) is the unique absolute minimizer of I in $\mathcal{A}_p^{rad}$ for $1 \leqslant p < 3$. The nontrivial minimizers in $\mathcal{A}_p^{rad}$ for $\lambda > \lambda_{cr}$ and $1 \leqslant p < 3$ have a point discontinuity at the origin corresponding to the formation of a hole, or cavity, of radius $r_\lambda(0)$. This is a multi-dimensional example of the Lavrentiev phenomenon (see (6.2)). For developments of these results see Sivaloganathan [46,47] and Stuart [48]. (An analysis in two dimensions along similar lines gives rise to the existence of cavitating radial minimizers for appropriate strictly polyconvex stored-energy functions; when considered as plane strain deformations of three-dimensional bodies these minimizers have a line discontinuity.) It is not known whether for $1 \leqslant p < 3$ the absolute minimum of I in $\mathcal{A}_p$ is attained, and if so whether there exists a radial minimizer. If for some λ the minimum is attained by some $u \not\equiv \lambda x$ then by rescaling and patching together u one can construct infinitely many such minimizers, with more and more finely distributed patterns of holes (see Ball [7], Ball & Murat [14]).

Cavitation is a well known fracture mechanism in both polymers (Gent & Lindley [27], Denecour & Gent [19], Gent & Park [28]) and metals (Hancock & Cowling [32], Needham, Wheatley & Greenwood [40]).

There is a large literature concerning examples of singular minimizers in the multi-dimensional calculus of variations, inspired by the examples of de Giorgi [18], Giusti &

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