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Published on: 01 Jan 1989 - Asymptotic Analysis (IOS Press) Topics: Relaxation (approximation) and Variational principle

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THE RELAXATION OF FUNCTIONALS WITH SURFACE ENERGIES

Ву

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IMA Preprint Series # 491
February 1989

The relaxation of functionals with surface energies

David Kinderlehrer and Giorgio Vergara - Caffarelli

Dedicated to the memory of Hans Lewy

1 Introduction

Consider a functional of the form

$$E(u) = \int_{\Omega} W(\nabla u) dx + \int_{\partial \Omega} \tau(\nabla u, u, v) dS, \quad u \in C^{1}(\overline{\Omega}; \mathbb{R}^{m}), \quad (1.1)$$

where $\Omega \subset \mathbb{R}^n$ is a domain with smooth boundary $\partial \Omega$ and outward normal ν , and W and τ are continuous functions. The distinguishing feature of E(u) here is that the surface term is permitted to depend on ∇u , the gradient of u. Our interest is to understand the relationship between the bulk energy and the superficial energy and the influence of the latter on possible extremals.

Suppose we have in hand a smooth u stationary for (1.1), namely,

$$\delta E(u) = 0, \qquad (1.2)$$

or, with $S(F) = \partial W/\partial F$ and $F = \nabla u$,

$$\int\limits_{\Omega} S(F) \cdot \nabla \zeta \; dx \; + \; \int\limits_{\partial} \left\{ \tau_F(F, u, v) \cdot \nabla \zeta \; + \; \tau_u(F, u, v) \cdot \zeta \right\} \; dS \; = \; 0 \; , \eqno(1.3)$$

$$\zeta \; \in \; C^1(\overline{\Omega} \; ; \mathbb{R}^m) .$$

¹ This research was supported by the NSF and the ASOFR under DMS 87 1881 and by the Universitá di Trento.

Seeking the Euler equations of (1.2) or (1.3) and keeping in mind that the choices of ζ and $\partial \zeta / \partial v$ are independent on $\partial \Omega$, we find that

$$-\operatorname{div} S(F) = 0 \qquad \text{in } \Omega \qquad (1.4)$$

$$S(F)v - \operatorname{div}_{\tan} \tau_F + \tau_u = 0 \qquad \text{on } \partial\Omega \qquad (1.5)$$

$$\tau_{FV} = 0 \qquad \text{on } \partial\Omega \qquad (1.6)$$

$$S(F)v - div_{tan}\tau_F + \tau_u = 0 \qquad \text{on } \partial\Omega$$
 (1.5)

$$\tau_{\rm F} v = 0 \qquad \qquad \text{on } \partial \Omega \tag{1.6}$$

where div_{tan} τ_F denotes the tangential divergence of τ_F .

We now wish to recount a suggestion of De Giorgi concerning the interpretation of (1.6). It may be expressed by writing

$$\frac{d}{d\lambda}f(\lambda) \Big|_{\lambda = 0} = \frac{d}{d\lambda}\tau(F + \lambda \xi \otimes \nu, u, v) \Big|_{\lambda = 0} = \tau_F(F, u, v) \cdot \xi \otimes \nu = 0$$
for all $\xi \in \mathbb{R}^m$.

So in particular, if τ is rank-one convex, then $f(\lambda)$ is convex and its derivative vanishes only at a minimum value. Thus

$$\tau(F,u,v) = \inf_{a \in \mathbb{R}^m} \tau(F_{tan} + a \otimes v,u,v)$$

$$F_{tan} = F - Fv \otimes v.$$
(1.7)

In conclusion, what De Giorgi has brought to light is that a stationary point of the functional seeks the minimum value of τ in the normal direction for a given value of the tangential gradient. Our aim in this note is to illustrate how this property is manifested in the relaxed functional for E and in its possible Young measure minimizers, both of which arise when W and τ are not quasiconvex.

We are aware of some recent work in this subject. Ball and Marsden consider functionals of the form (1.1), where τ does not depend on ∇u , [4]. They raise the issue of stability of solutions, illustrating that a necessary condition for a minimum involves both W and τ at the boundary. It will be readily apparent that the dependence of τ on ∇u makes the scaling so fruitfully employed in [4] very difficult in our case. Ball and Marsden also discuss dynamical stability. Fonseca is concerned with generalizations of the Maxwell rule and certain types of defects observed in crystals, [17]. We return to this topic in §8

and §9. Surface interactions are also discussed in [25]. In addition, we mention a recent work of Virga about liquid crystal droplets [29]. A general theory of the mechanical nature of superficial interaction is under development by Gurtin [18]. In the situation where the surface term is more properly interpreted as a loading, we refer to Gurtin and Spector [19] and Spector [26,27].

We might begin by introducing two simple examples. Consider the case where τ arises from a constant hydrostatic pressure p, so m = n = 3 and

$$p \int\limits_{\Omega} det \; \nabla u \; dx \;\; = \;\; \int\limits_{\partial \Omega} \tau(F,u,\nu) \; dS \;\; . \label{eq:partial}$$

For an invertible square matrix A, let us call

$$A^* = \det A A^{-T},$$

its adjugate or classical adjoint. With this notation,

$$\tau(F,u,v) = \frac{p}{3}F^* \cdot u \otimes v. \qquad (1.8)$$

it is easily verified that $\tau(F, u, v) = \tau(F + a \otimes v, u, v)$, so τ does not depend on the normal derivative and (1.6) is satisfied identically for all u.

As another example, consider a scalar valued u and

$$E(u) = \frac{1}{2} \int_{\Omega} |\nabla u|^2 dx + \frac{1}{2} \int_{\partial \Omega} (\frac{\partial u}{\partial v} - 1)^2 dS . \qquad (1.9)$$

Examination of the first variation leads to the system

$$\Delta u = 0 \qquad \text{in } \Omega$$

$$\frac{\partial u}{\partial v} = 0 \qquad \text{on } \partial \Omega$$

$$\frac{\partial u}{\partial v} = 1 \qquad \text{on } \partial \Omega,$$
(1.10)

which is inconsistent. We shall discuss a possible interpretation of this later.

In our subsequent discussion we shall always assume that

W and τ are continuous functions of their arguments and

$$W(A,\xi,x) \geq 0 \qquad \text{for } (A,\xi,x) \in \mathbb{M} \times \mathbb{R}^m \times \mathbb{R}^n , \qquad (1.10)$$

$$\tau(A,\xi,v) \geq 0 \qquad \text{for } (A,\xi,v) \in \mathbb{M} \times \mathbb{R}^m \times \mathbb{S}^{n-1} ,$$

where M denotes $m \times n$ matrices. This amounts to assuming that possible null-lagrangians like (1.8) are expressed as integrals over Ω which are dominated by the bulk energy density, and that the remaining surface energy densities are cooperative. For technical simplicity we shall not impose the kinematical constraint that det A > 0 when n = m. Let us set

$$\mathcal{E}(\mathbf{u}) = \int\limits_{\Omega} \mathbf{W}(\nabla \mathbf{u}, \mathbf{u}, \mathbf{x}) \, d\mathbf{x} + \int\limits_{\partial \Omega} \tau(\nabla \mathbf{u}, \mathbf{u}, \mathbf{v}) \, d\mathbf{S} , \quad \mathbf{u} \in \mathbf{C}^{1}(\overline{\Omega}; \mathbb{R}^{m}) \quad (1.12)$$

2 The relaxed problem

The quasiconvexification of W, or its quasiconvex minorant, is given by

$$W^{\#}(A,\xi,a) = \inf_{C} \frac{1}{|D|} \int_{D} W(A + \nabla \zeta(x),\xi,a) dx$$
, (2.1)

where $C = C_0^1(D)$ and $D \subset \mathbb{R}^n$ is a bounded domain with $|\partial D| = 0$. By (1.11), $W^\# \ge 0$. It is well known that $W^\#$ is quasiconvex and continous, cf. Dacorogna [6,7]¹, and that it is independent of D, cf. Ball and Murat [3]. The reader is reminded of Morrey's Theorem that the functional

$$\Phi(\mathbf{u}) = \int_{\Omega} \varphi(\nabla \mathbf{u}) \ d\mathbf{x}$$

is lower semi-continuous with respect to weak* convergence in $H^{1,\infty}(\Omega)$ when φ is continuous and quasiconvex [22,23]. Moreover, it is possible to show that for many functions W(A) and suitable admissible classes A,

$$\inf_{A} \int_{\Omega} W(\nabla u) dx = \inf_{A} \int_{\Omega} W^{\#}(\nabla u) dx.$$

We refer to [3,5,6,7,15,16] for a discussion of this and related points. For this reason the functional defined by W[#] is often called the relaxed functional.

In order to determine $\inf_A \mathcal{E}(u)$, we are led to discuss the relaxation of the superficial energy whose integrand is τ . Recall that we assume that τ is continuous. For a fixed $v \in S^{n-1}$, let $D' \subset \{x \cdot v = 0\}$ be a domain and let dx' denote the (n-1)-Lebesgue measure on D'. By $D' \times (-r,r)$, r > 0, we abbreviate the name of the set

¹ The infmum of continuous functions, $W^{\#}$ is upper semicontinuous. The appropriate line of reasoning in the present situation is upper semicontinuous \Rightarrow quasiconvex \Rightarrow rank one convex \Rightarrow (locally Lipschitz) continuous.

$$\{x \in \mathbb{R}^n: x' = (1 - v \otimes v)x \in D' \text{ and } |x \cdot v| < r\}.$$

Let [E] denote the n-1 dimensional Lebesgue measure of E. We define

$$\tau^{\#}(F,\xi,\nu) = \inf_{C'} \frac{1}{[D']} \int_{D'} \tau(F + \nabla \zeta,\xi,\nu) \, dx', \quad (F,\xi,\nu) \in \mathbb{M} \times \mathbb{R}^m \times \mathbb{S}^{n-1},$$

$$C' = C_0^1(D' \times (-r,r)).$$
(2.2)

We always suppose that $[\partial D'] = 0$. Clearly $\tau^{\#} \ge 0$ and is independent of r > 0. Precisely as in [3], it is independent of D', and analogously to [6,7] it is quasiconvex.

We refer to the functional

$$\mathcal{E}^{\#}(\mathbf{u}) \ = \ \int\limits_{\Omega} \mathbf{W}^{\#}(\nabla \mathbf{u}, \mathbf{u}, \mathbf{x}) \ d\mathbf{x} \ + \ \int\limits_{\partial \Omega} \tau^{\#}(\nabla \mathbf{u}, \mathbf{u}, \mathbf{v}) \ d\mathbf{S} \ , \ \mathbf{u} \ \in \ \mathbf{C}^{1}(\overline{\Omega}\,; \mathbb{R}^{m}), \ (2.3)$$

as the relaxed functional of \mathcal{E} . Our first objective is to prove¹

THEOREM 2.1 Let \mathcal{E} and $\mathcal{E}^{\#}$ be given by (1.12) and (2.3) and assume the continuity and positivity hypotheses (1.11) about W and τ . Then

$$\inf_{C^{1}(\overline{\Omega})} \mathcal{E}(u) = \inf_{C^{1}(\overline{\Omega})} \mathcal{E}^{\#}(u) = \inf_{H^{1}, \infty(\Omega)} \mathcal{E}^{\#}(u). \tag{2.4}$$

It will be part of the theorem to show that the last term in (2.4) is defined.

3 The tangential property of $\tau^{\#}$

The connection between the relaxation (2.4) and the formal discussion which gave rise to (1.7) is given via the density

¹ In the symbols for function spaces, we shall frequently suppress mention of the range space.

$$\tilde{\tau}$$
 $(F,\xi,\nu) = \tilde{\tau}$ $(F_{tan},\xi,\nu) = \inf_{y \in \mathbb{R}^3} \tau(F+y \otimes \nu,\xi,\nu)$ (3.1)
 $F_{tan} = F(1-\nu \otimes \nu)$.

For $\tilde{\tau}$ we have two ways of defining its quasiconvex minorant, either by

$$\tilde{\tau}_{1}^{\#}(F,\xi,v) = \inf_{C'} \frac{1}{[D']} \int_{D'} \tilde{\tau}(F + \nabla \zeta, \xi, v) dx'$$

or

It is elementary to check that these are equal, so we may speak of $\tilde{\tau}$ # unambiguously. Now $\tilde{\tau}$, the infimum of continuous functions, may be only upper semicontinuous, and therefore perhaps likewise for $\tilde{\tau}$ #. However, this issue, and that of the tangential nature of τ # is resolved in the next proposition.

PROPOSITION 3.1 With $\tilde{\tau}$ defined by (3.1),

$$\tilde{\tau} * (F,\xi,v) = \tau * (F,\xi,v)$$
. (3.2)

Proof. Since $\tilde{\tau} \leq \tau$, it is obvious that $\tilde{\tau}^{\#} \leq \tau^{\#}$. Given (F,ξ,ν) , let $\epsilon > 0$ and choose $\zeta \in C_0^1(D' \times (-r,r))$, where D' is a smooth domain, such that

$$\int_{D'} \tilde{\tau}(F + \nabla \zeta, \xi, v) dx' \leq \tilde{\tau} * (F, \xi, v)[D'] + \varepsilon.$$
 (3.3)

First note that since $\tilde{\tau}$ depends only on F_{tan} , we may assume in (3.3) that

$$\frac{\partial \zeta}{\partial v} = 0 \quad \text{for} \quad |x_n| < \frac{1}{2}r, \quad x' \in D'. \tag{3.4}$$

Secondly, any $\zeta \in C_0^1(D' \times (-r,r))$ may be approximated together with its gradient uniformly by piecewise affine functions. Combining this with the fact that $\tilde{\tau}$ is *upper semicontinuous*, we may assume that the ζ in (3.3) is piecewise affine and satisfies (3.4). Thus, we may write

$$D' = \bigcup_{i=1}^{M} D_i' \cup N$$
, $[N] = 0$, where $\nabla_{tan} \zeta = \nabla \zeta = A_i'$ in D_i' , $i = 1, ..., M$,

and the A_i are constant matrices.

Choose $y_i \in \mathbb{R}^m$ such that

$$|\tilde{\tau}(F + A_i, \xi, \nu) - \tau(F + A_i + y_i \otimes \nu, \xi, \nu)| < \frac{\varepsilon}{M}.$$
 (3.5)

Define a piecewise affine function ψ in $D' \times (-r,r)$ with

$$\nabla \psi = y_i \otimes v$$
 in D_i , $i = 1,...,M$, and $\psi = 0$ for $i \times_n i = r$.

Let $\eta \in C_0^1(D')$ be a scalar cut-off function for D'. Consider $\eta \psi$ so that

$$\nabla(\eta\psi) = \eta\nabla\psi + \psi\otimes\nabla\eta = \eta\nabla\psi$$
 on D'.

This permits us to compute that

$$\Big| \int_{D'} \tau(F + \nabla \zeta + \nabla (\eta \psi), \xi, \nu) \, dx' - \int_{D'} \tau(F + \nabla \zeta + \nabla \psi, \xi, \nu) \, dx' \, \Big| =$$

$$\Big| \int\limits_{D'} \tau(F + \nabla \zeta + \eta \nabla \psi, \xi, \nu) \, dx' - \int\limits_{D'} \tau(F + \nabla \zeta + \nabla \psi, \xi, \nu) \, dx' \, \Big| < \epsilon,$$

when supp $(1 - \eta)$ is small enough.

Finally, we may calculate that

$$\int_{D'} \tilde{\tau}(F + \nabla \zeta, \xi, \nu) dx' = \sum_{i=1}^{M} \int_{D'_{i}} \tilde{\tau}(F + A'_{i}, \xi, \nu) dx'$$

$$= \sum_{i=1}^{M} \tilde{\tau}(F + A'_{i}, \xi, \nu) [D'_{i}]$$

$$\geq \int_{D'} \tau(F + \nabla \zeta + \nabla \psi, \xi, \nu) dx' - \epsilon$$

$$\geq \int_{D'} \tilde{\tau}(F + \nabla \zeta + \nabla (\eta \psi), \xi, \nu) dx' - 2\epsilon$$

$$\geq \tau^{\#}(F, \xi, \nu) [D'] - 2\epsilon. \qquad QED$$

From the proposition, we conclude that $\mathcal{E}^{\#}$ is defined for $u \in H^{1,\infty}(\Omega)$. Now for any $u \in H^{1,\infty}(\Omega)$, we may find a sequence $u_{\varepsilon} \in C^{1}_{n}(\overline{\Omega})$ such that

$$\begin{array}{lll} u_{\epsilon} \, \to \, u & \text{uniformly in } \, \overline{\Omega} \,\,, \\ \nabla u_{\epsilon} \, \to \, \nabla u & \text{pointwise a.e. in } \, \Omega, \\ \nabla_{tan} u_{\epsilon} \, \to \, \nabla_{tan} u & \text{pointwise a.e. in } \, \partial \Omega, \quad \text{and} \\ \sup \Omega \, |\nabla u_{\epsilon}| \, + \, \sup_{\partial \Omega} |\nabla_{tan} u_{\epsilon}| \, \leq \, \text{const.} \end{array}$$

For example, u_ϵ may be found by convolution. By the continuity of $W^\#$ and $\tau^\#$ we conclude immediately that

$$\mathcal{E}^{\#}(u_{\epsilon}) \ \rightarrow \ \mathcal{E}^{\#}(u)$$

and thus that

$$\inf C^{1}(\overline{\Omega} \mathcal{E}^{\sharp}(u) = \inf H^{1,\infty}(\Omega) \mathcal{E}^{\sharp}(u),$$

which establishes the last equality of (2.4).

The formulas (3.1) and (3.2) show that

$$\tau^{\#}(F,\xi,v) = \tau^{\#}(F_{tan},\xi,v)$$
 (3.6)

This imples that $\tau^{\#}$ is generally different from τ even when τ is convex in A.

4 Approximation

We collect a few items about approximation, much of which is implicit in the literature.

LEMMA 4.1 Let $(F,\xi,a) \in \mathbb{M} \times \mathbb{R}^m \times \mathbb{R}^n$ and $D \subset \mathbb{R}^n$ with $|\partial D| = 0$. Given $\delta > 0$, there is a sequence $\zeta_h \in C_0^1(D)$ such that

$$\zeta_h \ \to \ 0 \quad \ \ \mbox{in} \ \ H^{1,\infty}(\Omega) \ \mbox{weak*} \ \mbox{and}$$

$$\int_{D} W(F + \nabla \zeta_{h}, \xi, a) dx \leq W^{\#}(F, \xi, a) |D| + \delta.$$
 (4.1)

Proof. First choose any $\zeta \in C_0^1(D)$ such that

$$\int\limits_{D} W(F + \nabla \zeta, \, \xi, \, a) \, dx \quad \leq \quad W^{\#}(F \, , \, \xi, \, a) \mid D \mid \, + \, \, \delta \, \, .$$

The collection of sets $\{c+\epsilon \ \overline{D}: c\in \overline{D} \text{ and } \epsilon \leq 1/h \}$ for each integer h form a cover of \overline{D} in the sense of Vitali, so we may find a finite or countable subcover $\{c_i+\epsilon_i \ \overline{D}\}$ which is pairwise disjoint such that

$$\overline{D} = \bigcup \{c_i + \varepsilon_i \ \overline{D}\} \cup N, \ |N| = 0,$$

so in particular $\sum_{i} (\epsilon_{i})^{n} = 1$.

Let us define

$$\zeta_h(x) = \begin{cases} \epsilon_i \zeta(\frac{x - c_i}{\epsilon_i}) & \text{if } x \in c_i + \epsilon_i D \\ 0 & \text{if } \text{otherwise.} \end{cases}$$

We compute that

$$\int_{D} W(F + \nabla \zeta_{h}, \xi, a) dx = \sum_{i} \int_{c_{i} + \epsilon_{i}D} W(F + \nabla \zeta_{h}, \xi, a) dx$$

$$= \sum_{i} \int_{c_{i} + \epsilon_{i}D} W(F + \nabla \zeta(\frac{x - c_{i}}{\epsilon_{i}}), \xi, a) dx$$

$$= \sum_{i} (\epsilon_{i})^{n} \int_{D} W(F + \nabla \zeta(z), \xi, a) dz$$

$$= \int_{D} W(F + \nabla \zeta(z), \xi, a) dz$$

$$\leq W^{\#}(F, \xi, a) |D| + \delta. \qquad QED$$

The novelty, if any, in the theorem below is that we allow dependence on $\,u\,$ and $\,x\,$ and the integrand $\,W\,$ is assumed to be only continuous.

THEOREM 4.2 Let $u \in C^1(\overline{\Omega})$ with Ω a Lipschitz domain. Given $\delta > 0$, there is a sequence $w_h \in C^1_0(\Omega)$ such that

$$w_h \rightarrow 0$$
 in $H^{1,\infty}(\Omega)$ weak* and

$$\int\limits_{\Omega}W(\nabla(u+w_h),u+w_h,x)\,dx \quad \leq \quad \int\limits_{\Omega}W^{\#}(\nabla u,u,x)\,dx \quad + \;\delta\;. \eqno(4.2)$$

Proof. We proceed in steps.

Step 1. Replacement by affine functions. Let us recall that given a positive integer h, we may find a function $v_h = v$ and a domain $\Omega_{oh} = \Omega_o$ such that

$$\begin{split} &\|\,v - u\,\|_{H^{1,\infty}(\Omega)} \, < \, \frac{1}{h} \,\,, \\ &v = \, u \quad \text{on} \ \partial\Omega, \\ &\{x: \, \operatorname{dist}(x,\!\partial\Omega) \, > \, \frac{1}{h} \,\,\} \, \subset \, \Omega_o \, \subset \subset \, \Omega, \quad \text{and} \\ &v \,\,\Big|_{\,\Omega_O} \quad \text{is piecewise affine.} \end{split} \tag{4.3}$$

Hence given $\epsilon > 0$, to be determined later, and the δ of (4.2), we may choose v and Ω_o so that

$$\left| \int_{\Omega} W^{\#}(\nabla v, v, x) dx - \int_{\Omega} W^{\#}(\nabla u, u, x) dx \right| < \varepsilon , \quad (4.4)$$

and

$$\int_{\Omega} W^{\#}(\nabla v, v, x) dx < \frac{1}{2} \delta, \qquad (4.5)$$

To check (4.3) - (4.5), we refer to Ekeland and Temam [8] p.317, for example. Then we may write

$$\Omega_0 = \bigcup_{i=1}^M \Omega_i \cup N, |N| = 0,$$
 where

 $\nabla v \mid_{\Omega_i} = A_i$, a constant matrix, i = 1,...,M, and also

$$\int_{\Omega_0} W^{\#}(\nabla v, v, x) dx = \sum_{i=1}^{M} \int_{\Omega_i} W^{\#}(A_i, v, x) dx. \qquad (4.6)$$

Note that throughout the remainder of the proof, v(x) is a known continuous function.

Step 2. Application of LEMMA 4.1 and scaling. Let D denote the unit cube in \mathbb{R}^n . Fix i and set $A=A_i$. By the definition of the Riemann integral, given $\varepsilon>0$, there is a $\lambda_{\varepsilon}>0$ such that whenever

$$\Omega_i \ = \ \bigcup \ \{a_s+\lambda_sD\ \} \cup N_i \ , \ |N_i| = 0 \quad \text{ and } \quad \left\{a_s+\lambda_sD\right\}$$
 pairwise disjoint with $\lambda_s<\lambda_\epsilon$, then

$$\left| \int_{\Omega_{i}} W^{\#}(A_{i},v,x) dx - \sum W^{\#}(A,v(a_{s}),a_{s}) |\lambda_{s}D| \right| < \epsilon.$$
 (4.7)

Given $a\in\Omega_0,$ by LEMMA 4.1 there is a $\,\zeta=\zeta_a\in\,C^1_0(D)\,$ such that

$$\sup |\zeta| < \frac{1}{h} \qquad \text{and} \qquad$$

$$\int\limits_{a}W(A+\nabla\zeta,v(a),a)\;dx\;\;\leq\;\;W^{\#}(A,v(a),a)\;\;+\;\;\gamma\;,$$

where y will be chosen later.

We now scale by setting

$$\zeta_{\lambda}(z) = \zeta_{a,\lambda}(z) = \lambda \zeta(\frac{z}{\lambda})$$

which has the properties

Now W is uniformly continuous on compact sets of its arguments, so by (4.8) we may find λ so small that

$$\int_{a+\lambda D} \left| W(A + \nabla \zeta_{\lambda}, v + \zeta_{\lambda}, x) - W(A + \nabla \zeta_{\lambda}, v(a), a) \right| dx \leq \gamma |\lambda D|.$$

Hence there is a $\lambda(a) \leq \lambda_{\epsilon}$ such that

whenever $\lambda \leq \lambda(a)$.

Step 3. Vitali covering. The sets $\{a + \lambda \ \overline{D} : \lambda \le \lambda(a)\}$ form a cover of Ω_i in the sense of Vitali, hence we may find a countable or finite subcollection $\{a_s + \lambda_s D\}$ such that $a_s + \lambda_s D$ are pairwise disjoint and

$$\Omega_i = \bigcup \{a_s + \lambda_s D\} \cup N_i, |N_i| = 0.$$

Thus with $\zeta_s = \zeta_{a_s; \lambda_s}$,

$$\sum_{a_s + \lambda D_s} \int_{\mathbf{D}_s} W(\mathbf{A} + \nabla \zeta_s, \mathbf{v} + \zeta_s, \mathbf{x}) \, d\mathbf{x} \leq \sum_{\mathbf{A}_s} (W^{\#}(\mathbf{A}, \mathbf{v}(a_s), a_s) + 2\gamma) \, |\lambda D|$$

$$\leq \int_{\Omega_s} W^{\#}(\mathbf{A}, \mathbf{v}(\mathbf{x}), \mathbf{x}) \, d\mathbf{x} + 2\gamma + \varepsilon. \quad (4.9)$$

Since the number of points $\{a_s\}$ which occur in the sum may be infinite, we cannot control the gradient of the function defined as ζ_s in $a_s + \lambda_s D$, that is, the numbers $C(a_s)$ in (4.8). Hence, choose a k > 0 such that

$$\sum_{s>k} \int_{a_s + \lambda D_s} W(A, v, x) dx < \varepsilon$$

and set

$$\zeta_i(x) \ = \ \left\{ \begin{array}{ccc} \zeta_s(x) & x \in \ a_s + \lambda_s D, \ s < k \\ 0 & \text{otherwise} \end{array} \right. .$$

Then

$$\int\limits_{\Omega_{\mathbf{i}}} W(A + \nabla \zeta_{\mathbf{i}}, v + \zeta_{\mathbf{i}}, x) \, dx \leq \int\limits_{\Omega_{\mathbf{i}}} W^{\#}(A, v, x) \, dx + 2\gamma + 2\varepsilon. \quad (4.10)$$

Step 4. Assembly and boundary condition Let us set

$$\zeta(x) \ = \ \left\{ \begin{array}{ll} \zeta_i(x) & x \in \ \Omega_i \\ 0 & \text{otherwise} \end{array} \right.$$

Then from (4.10) we have the estimate

$$\int\limits_{\Omega_0}W(\nabla v+\nabla\zeta,\,v+\zeta,x)\,\mathrm{d}x \ \leq \ \int\limits_{\Omega_0}W^\#(A,v,x)\,\mathrm{d}x \ + \ 2(\gamma+\epsilon)M\ , \ \ (4.11)$$

with

$$\sup |\zeta| < \frac{1}{h}$$
.

To complete the demonstration, define $w = w_h$ by

$$u + w = v + \zeta$$

and choose
$$2(\gamma + \epsilon)M < \frac{1}{2}\delta$$
. QED

Here is an example of an application of the preceding theorem, whose verification is left to the reader.

COROLLARY 4.3 Let Ω be a Lipschitz domain and $u_0 \in H^{1,\infty}(\Omega)$ be given. Then

$$\inf_A \int_{\Omega} W(\nabla u, u, x) dx = \inf_A \int_{\Omega} W^{\#}(\nabla u, u, x) dx$$

where

$$A = \left\{ v \in H^{1,\infty}(\Omega): v = u_0 \text{ on } \partial\Omega \right\}.$$

We shall require an analogous approximation for the surface term.

THEOREM 4.4 Let $D' \subset \mathbb{R}^{n-1}$ be a Lipschitz domain, $v \in C^o(D', \mathbb{S}^{n-1})$, and $u \in C^1(\overline{D}')$. Given $\delta > 0$, there is a sequence $\zeta_h \in C^1_0(D' \times (-r,r))$ such that

$$\begin{split} &\zeta_h \to 0 \qquad \text{in} \qquad H^{1,\infty}(D'\times (-r,r)) \ \textit{weak*} \ \textit{and} \\ &\int_D \tau(\nabla(u+\zeta_h), \ u+\zeta_h, \ v) \ dx' \ \leq \ \int_D \tau^\#(\nabla u, \ u \ , \ v) \ dx' \ + \ \delta \ . \end{aligned} \tag{4.12}$$

The proof is essentially identical to that of Theorem 4.2 and is omitted.

5 Proof of THEOREM 2.1

In this section we prove THEOREM 2.1. It suffices to show that given $u \in C^1(\overline{\Omega})$ and $\delta > 0$, there is a $v \in C^1(\overline{\Omega})$ such that

$$\mathcal{E}(v) \leq \mathcal{E}^{\#}(u) + \delta.$$
 (5.1)

In view of THEOREMS 4.2 and 4.4, our major effort will be to give a "global" version of (4.12), one valid on $\partial\Omega$. We shall then connect the boundary and the bulk pieces of the functional.

Let $\{\Sigma_i\}$ be a countable collection of smooth submanifolds of $\partial\Omega$ such that the Σ_i are pairwise disjoint and

$$\partial \Omega = \bigcup \Sigma_i \cup N, \quad \int_N dS = 0.$$

Let $\varepsilon > 0$. We assume that $\{\Sigma_i\}$ has the additional property that there is a collection $\{\varphi_i\}$ of smooth functions and open sets $\{U_i\}$, $U_i \subset \mathbb{R}^n$, $U_i \cap \partial \Omega = \Sigma_i$, with

$$\begin{array}{ll} \phi\colon \ U_i \ \to \ D_i \times (-r_i,r_i) \ , & \ D_i \ \subset \ \mathbb{R}^{n-1}, \\ \\ \sum \ [D_i] \ \le \ 2 \ \text{area} \ \partial \Omega, \ \text{and} \quad \left| \ \text{Jac} \ \phi_i \ - \ 1 \ \right| \ < \ \epsilon. \end{array} \tag{5.2}$$

For our given $u \in C^1(\overline{\Omega})$, let $u_i(z) = u(\phi_i^{-1}(z))$ for $z \in D_i \times (-r_i, r_i)$. By Theorem 4.5, for each u_i we may choose ζ_{ih} with

$$\sup |\zeta_{ih}| \leq \frac{1}{h} \quad \text{and}$$

$$\int_{D_i} \tau(\nabla(u_i + \zeta_{ih}), u_i + \zeta_{ih}, \nu) \, dx' \leq \int_{D_i} \tau^{\#}(\nabla u_i, u_i, \nu) \, dx' + \varepsilon \, [D_i] \, .$$
(5.3)

In the remainder of the calculation, we will denote by K a constant whose value may vary from line to line but depends only on the function u, which is fixed, and $\partial\Omega$. From (5.2) and (5.3), we may estimate that

$$\begin{split} \sum_{i} \int_{D_{i}} \tau(\nabla(u_{i} + \zeta_{ih}), u_{i} + \zeta_{ih}, v) \; dx' \; & \leq \; \sum_{i} \int_{D_{i}} \tau^{\#}(\nabla u_{i}, u_{i}, v) \; dx' \; + \; 2\epsilon \; \text{area} \; \partial\Omega \\ \\ & \leq \; \frac{1}{1 - \epsilon} \sum_{i} \int_{D_{i}} \tau^{\#}(\nabla u_{i}, u_{i}, v) \; Jac\phi_{i} \; dx' \; + \; 2\epsilon \; \text{area} \; \partial\Omega \end{split}$$

$$\leq \frac{1}{1-\varepsilon} \sum_{i} \int_{\Sigma_{i}} \tau^{\#}(\nabla u, u, v) \, dS + 2\varepsilon \text{ area } \partial\Omega$$

$$\leq (1+2\varepsilon) \sum_{i} \int_{\Sigma_{i}} \tau^{\#}(\nabla u, u, v) \, dS + 2\varepsilon \text{ area } \partial\Omega$$

$$\leq \int_{\partial\Omega} \tau^{\#}(\nabla u, u, v) \, dS + \varepsilon K$$

And thus

$$\sum_{i} \int_{D_{i}} \tau(\nabla(u_{i} + \zeta_{ih}), u_{i} + \zeta_{ih}, \nu) \operatorname{Jac}\phi_{i} dx' \leq \int_{\partial \Omega} \tau^{\#}(\nabla u, u, \nu) dS + \epsilon K. \quad (5.4)$$

Analogous to our discussion of (4.10), choose k so large that

$$\sum_{i>k} \int_{\Sigma_i} \tau^{\#}(\nabla u, u, v) dS < \varepsilon$$
 (5.5)

and define the functions

$$\begin{array}{ll} \psi_h(x) \; = \; \left\{ \begin{array}{ccc} \zeta_{ih}(\phi(x)) & x \in \sum_i \;,\; i \leq k \\ 0 & \text{otherwise} \end{array} \right. \quad \text{and} \\ \\ \overline{\psi}_h(x) \; = \; \left\{ \begin{array}{ccc} \frac{\partial \zeta_{ih}(\phi(x))}{\partial \nu} & x \in \sum_i \;,\; i \leq k \\ 0 & \text{otherwise} \end{array} \right. \,. \end{array}$$

Since $\partial\Omega$ is smooth, this choice permits us to extend ψ_h to a function continuously differentiable in a neighborhood in Ω such that

$$\frac{\partial \psi_h}{\partial v} \; = \; \stackrel{\longleftarrow}{\psi_h} \qquad \quad \text{on } \partial \Omega \qquad \quad \text{and} \quad \sup_{\Omega} |\psi_h| \; < \; \frac{2}{h} \, .$$

From (5.4) and (5.5), we have the estimate

$$\int_{\partial\Omega} \tau(\nabla(\mathbf{u} + \psi_h), \mathbf{u} + \psi_h, \mathbf{v}) \, d\mathbf{x}' \leq \int_{\partial\Omega} \tau^{\#}(\nabla \mathbf{u}, \mathbf{u}, \mathbf{v}) \, d\mathbf{x}' + \varepsilon \, K. \tag{5.6}$$

Finally, we may choose wh from (4.2) such that

$$\int\limits_{\Omega} W(\nabla (u+w_h),u+w_h,x)\,dx \quad \leq \quad \int\limits_{\Omega} W^{\#}(\nabla u,u,x)\,dx \quad + \ \epsilon \ .$$

Now let us set

$$v = \eta(u + w_h) + (1 - \eta)(u + \psi_h) = u + \eta w_h + (1 - \eta)\psi_h$$
,

where $\,\eta\,$ is a cut-off function. Since both $\,w_h\,$ and $\,\psi_h\,$ converge uniformly to 0, we may choose $\,\eta\,$ and then $\,h\,$ so that

$$\mathcal{E}(v) \leq \mathcal{E}^{\#}(u) + \epsilon K$$
. QED

6 Parametrized measure minimizers

Suppose that $(u^k) \subset C^1(\overline{\Omega})$ is a minimizing sequence for $\mathcal{E}(u)$ which is bounded in $H^{1,\infty}(\Omega)$. After extraction of a subsequence, we may assume that there is a $u \in H^{1,\infty}(\Omega;\mathbb{R}^m)$ such that

$$u^k \rightarrow u \quad \text{in } H^{1,\infty}(\Omega;\mathbb{R}^m) \text{ weak*}.$$
 (6.1)

Indeed, slightly more is true, which shall be of use in our situation. The functions ∇u^k are continuous and bounded in $\Omega \cup \partial \Omega$, from which it follows that in addition to (6.1), there is a matrix $F(x) \in L^{\infty}(\partial \Omega; \mathbb{R}^m)$ such that

$$\nabla u^k \to F$$
 in $L^{\infty}(\partial\Omega;\mathbb{R}^m)$ weak* with $\nabla_{tan}u = F(1-\nu\otimes\nu)$. (6.2)

Although $\mathcal{E}(\mathbf{u})$ need not even be defined, owing to Theorem 2.1,

$$\mathcal{L}^{\#}(\mathbf{u}) = \lim_{k \to \infty} \mathcal{L}^{\#}(\mathbf{u}^k) = \lim_{k \to \infty} \mathcal{E}(\mathbf{u}^k) = \inf \mathcal{E}(\mathbf{v}).$$
 (6.3)

In evidence are a limit configuration u and a limit energy $\mathcal{E}^{\#}(u)$ with little apparent connection between them. This connection is provided by the Young measure or parametrized measure introduced by L. C. Young [30]. Its existence and properties have been noted in many places in various forms [1,2,5]. For an introduction to its use in differential equations we refer to Tartar [28].

Briefly, let $K \subset \mathbb{R}^m$ be compact such that supp $\nabla u^k \subset K$ for all k. Then there is a family of probability measures $(\mu_X)_{X \in \Omega} \subset M(K)$, the Radon measures on K, such that for any $\psi(A,x)$ continuous in A and integrable in x,

For example, since

$$\nabla u^k \rightarrow \nabla u$$
 in $L^{\infty}(\Omega)$ weak*,

$$\nabla u(x) \ = \ \int\limits_K \ A \ d\mu_x(A) \ , \ a.e. \ in \ \Omega.$$

Moreover, it is well known that any minor M(A) is weak* continous, so

$$M(\nabla u(x)) \ = \ \int\limits_K \ M(A) \ d\mu_X(A) \ , \ a.e. \ in \ \Omega.$$

More generally, regarding $F = \nabla u$ in Ω as well as on $\partial \Omega$,

$$M(F(x)) \ = \ \int\limits_K \ M(A) \ d\mu_x(A) \ , \ dx \ a.e. \ in \ \Omega \ \ and \ \ dS \ a.e. \ in \ \partial\Omega \ . \ (6.5)$$

For the minimizing sequence (u^k) there is an additional weak* continuous function owing to the lower semi-continuity of $\mathcal{E}^{\#}$.

LEMMA 6.1 Let $(u^k) \subset C^1(\overline{\Omega})$ be a minimizing sequence for $\mathcal{E}(u)$ such that

$$\nabla u^k \ \to \ F \qquad \qquad \text{in $L^\infty(\Omega) \cup L^\infty(\partial\Omega)$ weak*}.$$

Then

In particular,

$$\begin{split} W^\#(F(x),\!u(x),\!x) \;\; &=\;\; \int\limits_K \; W^\#(A,\!u(x),\!x) \; d\mu_X(A) \;, \;\; dx \;\; \text{a.e. in} \;\; \Omega \;\; \text{and} \\ \\ \tau^\#(F(x),\!u(x),\!v) \;\; &=\;\; \int\limits_K \; \tau^\#(A,\!u(x),\!v) \;\; d\mu_X(A) \;, \;\; dS \;\; \text{a.e. in} \;\; \partial\Omega \;. \end{split} \label{eq:power_power}$$

The statement (6.6) follows easily from (6.3); details are omitted. On the other hand, the functions ($W(\nabla u^k, u^k, x)$) and ($\tau(\nabla u^k, u^k, v)$) are bounded sequences which converge weak* to functions $\overline{W}(x)$ and $\overline{\tau}(x)$, respectively. It follows from the definition of the Young measure that

$$\overline{W}(x) \ = \ \int\limits_K \ W(A,u(x),x) \ d\mu_X(A) \ , \quad dx \ a.e. \ in \ \Omega \ and$$

$$\overline{\tau}(x) \ = \ \int\limits_K \ \tau(A,u(x),v) \ d\mu_X(A), \quad dS \ a.e. \ in \ \partial\Omega \ .$$

From (6.3),

$$\mathcal{E}^{\#}(u) = \int_{\Omega} \overline{W}(x) dx + \int_{\partial \Omega} \overline{\tau}(x) dx. \qquad (6.9)$$

This next result delineates the nature of the support of (μ_X). Its proof is analogous to Theorem 5.4 [5].

THEOREM 6.1 Let $(u^k) \subset C^1(\overline{\Omega})$ be a minimizing sequence for E(u) such that

$$\begin{array}{lll} u^k \to u & \text{in } H^{1,\infty}(\Omega) \text{ and} \\ \nabla u^k \to F & \text{in } L^{\infty}(\Omega) \cap L^{\infty}(\partial\Omega) \text{ weak*, and} \\ \text{supp } \nabla u^k \subset K, & K \text{ compact in } \mathbb{R}^m \,. \end{array}$$

Let (μ_X) be the parametrized measure determined by (∇u^k) . Then

$$\sup \mu_X \subset \{ A \in \mathbb{M} \colon W(A,u(x),x) = W^\#(A,u(x),x) \}, \text{ a.e. in } \Omega$$
 and
$$\sup \mu_X \subset \{ A \in \mathbb{M} \colon \tau(A,u(x),x) = \tau^\#(A,u(x),x) \}, \text{ a.e. on } \partial\Omega.$$

In particular,

$$\overline{W}(x) = \int\limits_K W^\#(A,u(x),x) \; d\mu_X(A) \;, \quad dx \; a.e. \; in \; \Omega$$
 and
$$\overline{\tau}(x) = \int\limits_K \tau^\#(A,u(x),v) \; d\mu_X(A), \quad dS \; a.e. \; in \; \partial\Omega \;.$$

Proof. Evaluating both sides of (6.9) gives that

$$\int_{\Omega} \left\{ \overline{W}(x) - W^{\#}(F,u(x),x) \right\} dx + \int_{\partial\Omega} \left\{ \overline{\tau}(x) - \tau^{\#}(F,u(x),x) \right\} dS = 0.$$

Now observe that

$$\overline{W}(x) \ = \ \int\limits_K \ W(A,u(x),x) \ d\mu_X(A) \ \geq \ \int\limits_K \ W^\#(A,u(x),x) \ d\mu_X(A) \ = \ W^\#(F,u(x),x)$$

and

$$\overline{\tau}(x) \ = \ \int\limits_K \tau(A, u(x), v) \ d\mu_x(A) \ \geq \ \int\limits_K \tau^\#(A, u(x), v) \ d\mu_x(A) \ \geq \ \tau^\#(F, u(x), v),$$

and hence equality holds. This proves both (6.11) and (6.10). QED

7 Elementary examples

Let us begin by returning to (1.9), which has the "inconsistent" equilibrium equations (1.10). For this functional, since u is scalar valued, we may write

$$\tau(a,v) = \frac{1}{2}(a\cdot v - 1)^2, \quad a \in \mathbb{R}^n.$$
 (7.1)

Thus

$$\widetilde{\tau}(a,v) \ = \ \inf{}_{t \in \ \mathbb{R}} \, \tau(a+tv,v) \ = \ \inf{}_{t \in \ \mathbb{R}} \, \tfrac{1}{2} \, (a\cdot v \ +t-1)^2 \ = \ 0 \; ,$$

so
$$\tilde{\tau}^{\#}(a,v) = \tau^{\#}(a,v) = 0$$
, for all $a \in \mathbb{R}^n$.

Consider a local situation, namely, $\Omega=\{\,x_n>0,\,|\,x\,|<1\},$ $\Gamma=\{\,x_n=0,\,|\,x\,|<1\},$ and

$$E(u) = \frac{1}{2} \int_{\Omega} |\nabla u|^2 dx + \frac{1}{2} \int_{\Gamma} (\frac{\partial u}{\partial v} - 1)^2 dx', \qquad (7.2)$$

 $\nu = -\,e_n$. Let $\,u^\epsilon(x) = -\,min\,(x_n,\epsilon),\,\, \epsilon > 0$. Then

$$u^{\epsilon} \rightarrow 0$$
 in $H^{1}(\Omega)$ as $\epsilon \rightarrow 0$,

although

$$\nabla u^{\varepsilon} = -e_n$$
 on Γ .

From this, it is easy to deduce that the minimizing Young measure $(\mu_{\boldsymbol{x}})$ has the form

$$\mu_{x} = \begin{cases} \delta_{0} & \text{if } x \in \Omega \\ \delta_{-e_{n}} & \text{if } x \in \Gamma \end{cases}$$
 (7.3)

Note that even though τ is convex, $\tau^{\#} \neq \tau$.

We next consider the functional

$$E(u) = \int_{\Omega} \varphi(\det \nabla u) \, dx + \int_{\partial \Omega} f(\det \nabla u) \, dS, \quad u \in C^{1}(\overline{\Omega}), \quad (7.4)$$

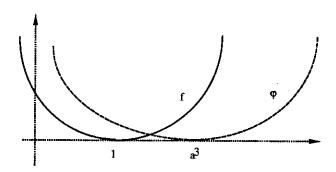
where ϕ and f are smooth convex functions, nonnegative, with

$$\varphi(a^3) = \inf \varphi = 0$$

$$f(1) = \inf f = 0,$$
(7.5)

for some $a \neq 0,1$. We assume that $\Omega \subset \mathbb{R}^3$.

and



Functions φ and f satisfying (7.5)

The equilibrium equations for (7.4) are inconsistent like (1.11). Let us establish directly that

$$\inf E(\mathbf{u}) = 0. \tag{7.6}$$

Let $\rho(x) = \operatorname{dist}(x,\partial\Omega)$, $x \in \Omega$, which is C^1 near $\partial\Omega$ under the assumption that $\partial\Omega$ is smooth. Note that

$$\nabla \rho = \nu$$
 on $\partial \Omega$.

Let $g^{\epsilon}(t)$, $t \in \mathbb{R}$, be a sequence of smooth functions such that

$$\begin{array}{lll} g^\epsilon(0) &=& 0, & g^\epsilon(t) &=& 0 & \text{ for } t \geq \epsilon, \text{ and} \\ \frac{dg^\epsilon}{dt}(0) &=& \sup \left| \frac{dg^\epsilon}{dt} \right| &=& \gamma\,, \end{array}$$

where y will be chosen later. Set

$$u^{\varepsilon}(x) = ax + g^{\varepsilon}(\rho(x))v(x), \qquad x \in \overline{\Omega}.$$
 (7.7)

Thus

$$\begin{split} \nabla u^{\epsilon} &= a\mathbf{1} \, + \, \frac{\mathrm{d}g^{\epsilon}}{\mathrm{d}t}(\rho) \, v \otimes v \, + \, g^{\epsilon} \nabla v \\ &= a\mathbf{1} \, + \, \gamma \, v \otimes v \qquad \qquad \text{on } \partial \Omega. \end{split}$$

Also,

$$\det \nabla u^{\varepsilon} = a^{2}(a+\gamma) = 1 \qquad \text{on } \partial \Omega \text{ for the choice}$$

$$\gamma = \frac{1}{a^{2}} - a.$$

For this choice of u^e, one checks that

$$E(u^\epsilon) \ = \ \int\limits_{supp} \phi(\det \nabla u^\epsilon) \; dx \ \to \ 0 \ as \ \epsilon \ \to \ 0.$$

Moreover, the Young measure determined by (u^ϵ) is $\,\delta_{F(x)}\,$ where

$$F(x) = \begin{cases} a1 & \text{if } x \in \Omega \\ a1 + (\frac{1}{a^2} - a)v \otimes v & \text{if } x \in \partial \Omega \end{cases}$$

It is of interest to compute the relaxed functional. With

$$\tau(A) = f(\det A),$$

we have that

$$\tilde{\tau}(A,v) = \inf_{y} f(\det(A + y \otimes v)).$$

Recall the formula

$$det(A + B) = det A + A* \cdot B + A \cdot B* + det B, A,B 3 \times 3$$
matrices,

where

$$C^* = \text{adjugate of } C = \left(\frac{1}{2} \epsilon_{ihk} \epsilon_{jrs} C_{hr} C_{ks}\right).$$

When det C \neq 0, C* = det C C^{-T} = $\frac{d}{dC}$ det C. Since $y \otimes v$ is of rank 1, $(y \otimes v)^* = 0$ and det $(y \otimes v) = 0$, so

$$\det (A + y \otimes v) = \det A + A^* \cdot y \otimes v = \det A + A^*v \cdot y.$$

It follows immediately that

$$\widetilde{\tau}(A,v) = \begin{cases} f(1) & \text{if} & A*v \neq 0 \\ f(0) & \text{if} & A*v = 0 \end{cases}$$

$$= \begin{cases} 0 & \text{if} & A*v \neq 0 \\ f(0) & \text{if} & A*v \neq 0 \end{cases}$$

Since the matrices A for which A*v = 0 are simply a subset of those of vanishing determinant, a closed nowhere dense set, the continuity of $\tau^{\#}$ insures us that

$$\tau^{\#}(A,v) = 0 \qquad \text{for all } A \in \mathbb{M}. \tag{7.8}$$

Hence the relaxed functional for (7.3) is

$$E^{\#}(u) = \int_{\Omega} \varphi(\det \nabla u) \, dx \qquad (7.9)$$

8 Some remarks about elastic crystals

We wish to address a few issues which illustrate the role of symmetry groups in the possible relaxation of a superficial density. We intend to investigate densities suggested by the constitutive theory for elastic crystals following Ericksen, cf. [9,10,11,12]. Discussions of the consequences of these ideas, for example, in the analysis of microstructural properties, are given in Ball and James [2], Ericksen [13], and James [20], for example, as well as Fonseca [16] and [5], cf. also [21]. The parametrized measure is a useful device in some of this work, although it may be only implicit in the discussion. The extension of these ideas to surface interaction has been developed by Parry [24] and Fonseca [17].

The relaxation which we discuss below has been determined by Fonseca [17]. Our approach is somewhat different since we already know that a possible $\tau^{\#}$ depends only on F_{tan} , although much of the technical manipulation may seem similar.

We set m=n=2 or 3. Let $\Omega\subset\mathbb{R}^n$ be a domain with smooth boundary Γ . We shall neglect any dependence on temperature. Let us assume, analogously to (1.11), that $W(A)\in C(\mathbb{M})$ and $\tau(A,\xi,\nu)\in C(\mathbb{M}\times\mathbb{R}^n\times\mathbb{R}^n)$ and satisfy

$$W(A) \ge 0 \qquad \text{for } A \in M \tag{8.1}$$

and

$$\tau(A,\xi,v) \ge 0$$
 for $(A,\xi,v) \in \mathbb{M} \times \mathbb{R}^n \times \mathbb{R}^n$, with $\tau(A,\xi,\lambda v) = \tau(A,\xi,v)$ when $\lambda > 0$.

Hypotheses on W:

$$W(QA) = W(A)$$
 for $Q \in SO(3)$ (frame indifference) (8.3) $W(AH) = W(A)$ for $H \in \mathbb{H}_{\Omega}$, (material symmetry)

where $\mathbb{H}_{\Omega} = LGL(\mathbb{Z}^3)L^{-1}$ is a conjugate group of $GL(\mathbb{Z}^3)$.

Hypotheses on τ :

$$\tau(QA,Q\xi,v) = \tau(A,\xi,v)$$
 for $Q \in SO(3)$ (frame indifference) (8.4) $\tau(AH,\xi,H^Tv) = \tau(A,\xi,v)$ for $H \in \mathbb{H}_{\Gamma}$, (material symmetry) (8.5)

where \mathbb{H}_{Γ} is a conjugate group of $GL(\mathbb{Z}^3)$, perhaps different from \mathbb{H}_{Ω} . Note that this is precisely the symmetry satisfied by (1.8), which is the determinant. Considerations at the level of the crystal lattice may be used to justify (8.3)₂ and (8.5). Let us set

$$\mathcal{E}(u) = \int\limits_{\Omega} W(\nabla u) \, dx + \int\limits_{\partial \Omega} \tau(\nabla u, u, v) \, dS \,, \quad u \in C^{1}(\overline{\Omega}) \,. \tag{8.6}$$

Our objective is to identify the functional $\mathcal{L}^{\sharp}(u)$ of (2.3). To this end we review briefly what is known about the bulk term. Introduce the function

$$\varphi(\det F) = \inf_{\det A = \det F} W(A), \tag{8.7}$$

which is Ericksen's sub-energy for W, [11]. Then, according to [5,16],

$$W^{\#}(A) = \phi^{**}(\det A), \qquad A \in M,$$
 (8.8)

where $\phi^{**}(t)$ is the convexification of $\phi(t)$. In fact, Fonseca shows that $(8.3)_2$ alone is sufficient for (8.8) to hold.

To define the quantity analogous to (8.7) for τ requires some care. As our subsequent demonstration will show, we came upon the characterization after deducing its principal properties. Provisionally, let us set

$$\sigma(F^*v,\xi,v) = \inf_{A^*v = F^*v} \tau(A,\xi,v),$$

where A^* denotes the adjugate of A, as usual. It turns out that it is relatively easy to show that σ depends only on the vectors F^*v and ξ . Anticipating this, set

$$\psi(F^*v, \xi) = \inf_{A^*v = F^*v} \tau(A, \xi, v).$$
(8.9)

This function plays the role of the subenergy (8.7) for τ .

THEOREM 8.1 Under the hypotheses (8.2) and (8.5) (material symmetry) about $\tau(A,\xi,v)$, let ψ be defined by (8.9). Then

$$\tau^{\#}(F,\xi,v) = \psi^{**}(F^{*}v,\xi),$$
 (8.10)

where ψ^{**} denotes the convexification of $\psi(a,\xi)$ in the variable a.

Thus the relaxed functional for (8.6) is

When, in addition, frame indifference is imposed, we shall show that

$$\sigma(F^*v,\xi,v) = \psi_0(|F^*v|,F^*\cdot\xi\otimes v,|\xi|), \qquad (8.12)$$

where ψ_0 is a function of the three scalars $|F^*v|$, $F^* \cdot \xi \otimes v$, and $|\xi|$.

COROLLARY 8.2 Under the hypotheses (8.2), (8.4), and (8.5) about $\tau(A,\xi,v)$, let ψ_0 be defined by (8.11). Then

$$\tau^{\#}(F,\xi,\nu) = \psi_{0}^{**}(|F^{*}\nu|, F^{*}\cdot \xi \otimes \nu, |\xi|)$$
 (8.13)

where ψ^{**} denotes the convexification of $\psi(\alpha,\beta,\gamma)$ with respect to the real variables (α,β) . Moreover ψ^{**} is increasing in α .

The first part of the proof will be directed towards showing that there is some function $f(a,\xi)$ which fulfills (8.10). We then show that $f=\psi^{**}$. There are a number of elementary facts about the group H we collect here. Proofs appear in the appendix to this section.

ELEMENTARY FACTS

a. Let $v \in S^2$. Then there are $M_k \in \mathbb{H}$ such that

$$\frac{\mathbf{M}_{\mathbf{k}}^{\mathrm{T}} \mathbf{v}}{|\mathbf{M}_{\mathbf{k}}^{\mathrm{T}} \mathbf{v}|} \to \mathbf{e}_{1} \qquad \text{as } \mathbf{k} \to \infty. \tag{8.14}$$

b. Let $a, n \in \mathbb{R}^3$ and $v \in \mathbb{S}^2$ with $a \cdot n = a \cdot v = 0$. Then there are $H_k \in \mathbb{H}$, $\lambda_k \in (0,1)$, and $v_k \in \mathbb{S}^2$ such that

$$1 + a \otimes n = \lim_{k \to \infty} ((1 - \lambda_k) \mathbb{1} + \lambda_k H_k), \quad v = \lim_{k \to \infty} v_k, \text{ and } H_k^T v_K = v_K.$$

$$(8.15)$$

c. Given $Q \in SO(2)$, there are vectors a_i , $n_i \in \mathbb{R}^2$ with $a_i \cdot n_i = 0$, i = 1,2,3, such that

$$Q = (1 + a_1 \otimes n_1)(1 + a_2 \otimes n_2)(1 + a_3 \otimes n_3).$$
 (8.16)

To check that $\tau^{\#}$ satisfies the symmetry condition (8.5) is easily accomplished by changing variables in the integral in (2.2).

LEMMA 8.3 Suppose that $a \cdot n = a \cdot v = 0$. Then

$$\tau^{\#}(A(1 + a \otimes n), \xi, v) = \tau^{\#}(A, \xi, v)$$
. (8.17)

Proof. Observe that the condition $a \cdot v = 0$ is the same as

$$(1 + a \otimes n)^{T} v = v.$$

It suffices to show that

$$\tau^{\#}(A(\mathbb{I} + a \otimes n), \xi, \nu) \leq \tau^{\#}(A, \xi, \nu), \tag{8.18}$$

for in (8.18) we may replace A by $A(1+a\otimes n)$ and $1+a\otimes n$ by $1-a\otimes n$ to obtain

$$\tau^{\#}(A,\xi,\nu) \leq \tau^{\#}(A(1+a\otimes n),\xi,\nu). \tag{8.19}$$

Suppose first that $H = 1 + p \otimes q \in H$ and $v \cdot p = 0$. Then by rank-one convexity of $\tau^{\#}$ and (8.2),

$$\tau^{\#}(A(1 + \lambda p \otimes q), \xi, \nu) \leq (1 - \lambda) \tau^{\#}(A, \xi, \nu) + \lambda \tau^{\#}(AH, \xi, \nu)$$

$$= (1 - \lambda) \tau^{\#}(A, \xi, \nu) + \lambda \tau^{\#}(AH, \xi, H^{T}\nu)$$

$$= \tau^{\#}(A, \xi, \nu) .$$

Hence by (8.19),

$$\tau^{\#}(A(\mathbb{1}+\lambda p\otimes q),\xi,\nu) = \tau^{\#}(A,\xi,\nu) \qquad \text{when} \quad p\cdot q = p\cdot \nu = 0$$
 and $0\leq \lambda \leq 1$. (8.20)

Given a, n, ν , choose a sequence H_k , λ_k , and ν_k satisfying (8.12). The result follows by continuity of $\tau^{\#}$.

LEMMA 8.4 Let F and A be 3×3 matrices satisfying

$$F^*v = A^*v \neq 0.$$
 (8.21)

Then there are a rotation Q with axis v, a simple shear $E = 1 + a \otimes n$, with $n \cdot v = 0$, and an $M \in H$ such that

$$A_{tan}M = F_{tan}MQE. (8.22)$$

 $M = 1 if F*v \cdot v \neq 0.$

Proof. First note that $(1 - v \otimes v)^* = v \otimes v$, so the hypothesis (8.21) is equivalent to

$$(F(1-v\otimes v))^* = (A(1-v\otimes v))^* \qquad \text{or}$$

$$F_{tan}^*v = A_{tan}^*v \qquad \text{or}$$

$$Ft_1 \wedge Ft_2 = At_1 \wedge At_2,$$

$$(8.23)$$

where (t_1,t_2,v) is an orthonormal basis. Inspecting the third components of these vectors, in the (t_1,t_2,v) coordinates, we have

$$F_{11}F_{22} - F_{12}F_{21} = A_{11}A_{22} - A_{12}A_{21},$$
 (8.24)

which we assume nonzero for the moment. Let

$$F' \ = \ \left(\begin{array}{ccc} F_{11} & F_{12} & 0 \\ F_{21} & F_{22} & 0 \\ 0 & 0 & 0 \end{array} \right) \ \text{and} \quad A' \ = \ \left(\begin{array}{ccc} A_{11} & A_{12} & 0 \\ A_{21} & A_{22} & 0 \\ 0 & 0 & 0 \end{array} \right)$$

so that

$$F_{tan} = (Ft_1,Ft_2,0) = F' + v \otimes f$$
, $f \cdot v = 0$, and $A_{tan} = (At_1,At_2,0) = A' + v \otimes a$, $a \cdot v = 0$.

By the factorization lemma [5], Proposition 3.4, A' = F'QE where Q is a rotation with axis ν and E = 1 + a \otimes n with a \cdot n = a \cdot ν = 0. Hence

$$A_{tan} = FQE + v \otimes a = (F_{tan} + v \otimes c)QE, \qquad (8.25)$$

for some c with $c \cdot v = 0$, after a little manipulation. Now compute that

$$A_{tan}*v = (F_{tan} + v \otimes c)*QE*v$$

with

$$QE*v = Q(1-n \otimes a)v = Qv = v,$$

or

$$A_{tan}*v = (F_{tan} + v \otimes c)*v$$
.

So from (8.23),

$$F_{tan}*v = (F_{tan} + v \otimes c)*v$$
.

Writing this as

$$\begin{pmatrix} F_{11} \\ F_{21} \\ F_{31} \end{pmatrix} \wedge \begin{pmatrix} F_{12} \\ F_{22} \\ F_{32} \end{pmatrix} = \begin{pmatrix} F_{11} \\ F_{21} \\ F_{31} + c_1 \end{pmatrix} \wedge \begin{pmatrix} F_{12} \\ F_{22} \\ F_{32} + c_2 \end{pmatrix}$$

and inspecting gives rise to the two equations

$$F_{11} c_2 - F_{12} c_1 = 0$$

$$F_{21} c_2 - F_{22} c_1 = 0,$$

which by our assumption that (8.24) does not vanish implies that c = (0,0). Using this in (8.25) gives that

$$A_{tan} = F_{tan} QE$$
.

The assumption about (8.24) is equivalent to $F^*v \cdot v \neq 0$. If $F^*v \cdot v = 0$, simply find an element M of H which is a permutation matrix such that $(FM)^*v \cdot v \neq 0$ and apply the preceding result to FM and AM. This is always possible if $F^*v \neq 0$. QED

PROPOSITION 8.5 Let A and F be matrices. If

$$F^*v = A^*v.$$

then

$$\tau^{\#}(F,\xi,v) = \tau^{\#}(A,\xi,v) .$$

Proof According to the previous lemma, $A_{tan}M = F_{tan}MQE$. By the elementary fact c., we may write

Q =
$$(1 + a_1 \otimes n_1)(1 + a_2 \otimes n_2)(1 + a_3 \otimes n_3) = E_1E_2E_3$$
, with $a_i \cdot n_i = a_i \cdot v = n_i \cdot v = 0$.

Hence

$$A_{tan}M = F_{tan}ME_1E_2E_3E$$
.

By LEMMA 8.3,

$$\tau^{\#}(A_{tan}M,\xi,\nu) = \tau^{\#}(F_{tan}M,\xi,\nu),$$

and in particular, replacing v by $M^{-T}v$, we obtain the conclusion.

QED

We may now begin to use the invariance and frame indifference to determine additional properties of $\tau^{\#}(A,\xi,\nu)$. First of all, there is a function $f(a,\xi,\nu)$ such that

$$\tau^{\#}(A,\xi,v) = f(A*v,\xi,v).$$

Given v, let $(M_k) \subset \mathbb{H}$ satisfy the conditions of elementary fact a. Then, noting that $M^* = M^{-T}$ for $M \in \mathbb{H}$,

$$\begin{split} f(A^*v,&\xi,v) &= f(A^*M_k^*M_k^Tv,&\xi,M_k^Tv) &= f(A^*v,&\xi,M_k^Tv) \\ &\to f(A^*v,&\xi,e_1) &\text{as } k \to \infty. \end{split}$$

Thus,

$$f = f(A*v,\xi)$$
.

Quasiconvexity of $\tau^{\#}$ implies that the function $f(a,\xi)$ is convex in a, as is well known.

Introduce

$$\sigma(F^*v, \xi, v) = \inf_{A^*v = F^*v} \tau(A, \xi, v)$$
.

For $M \in \mathbb{H}$,

$$\sigma(F^*v,\xi,v) = \inf_{A^*v = F^*v} \tau(AM,\xi,M^Tv)$$

$$= \inf_{(AM)*M^Tv = (FM)*M^Tv} \tau(AM,\xi,M^Tv)$$
$$= \sigma((FM)*M^Tv,\xi,M^Tv) = \sigma(F*v,\xi,M^Tv).$$

Once again by elementary fact a, we deduce that σ depends on ν only through $F^*\nu$, hence we may write

$$\psi(F^*v,\xi) = \sigma(F^*v,\xi,v) = \inf_{A^*v = F^*v} \tau(A,\xi,v). \tag{8.26}$$

Now we establish (8.10). Since $\psi \le \tau$, it is immediate that

$$\Psi^{**} \leq \tau^{\#} = f \leq \tau$$
. (8.27)

We must show the reverse inequality. From the definitions of ψ and $\tau^{\#}$, given F and $\epsilon>0$, we may choose an F_{ϵ} such that

$$\begin{array}{rcl} f(F_{\epsilon}^*\nu,\xi) & = & \tau^\#(F_{\epsilon},\xi,\nu) & \leq & \tau(F_{\epsilon},\xi,\nu) & \leq & \psi \left(F^*\nu,\xi\right) \, + \, \epsilon \, , \\ \\ & \text{with} & & F_{\epsilon}^*\nu & = & F^*\nu \, . \end{array}$$

As we have established in PROPOSITION 8.5,

$$\tau^{\#}(F,\xi,v) = \tau^{\#}(F_{\epsilon},\xi,v),$$

so

$$f(F^*v,\xi) \leq \psi(F^*v,\xi) + \varepsilon$$
,

hence,

$$f(F^*v,\xi) \leq \psi(F^*v,\xi)$$
.

In effect, $f(a,\xi) \le \psi(a,\xi)$ and is convex in a. Thus,

$$f(a,\xi) \le \psi^{**}(a,\xi)$$
. (8.28)

Combining (8.27) and (8.28), THEOREM 8.1 is proved. QED

Proof of COROLLARY 8.2. By frame indifference,

$$\psi(QA^*v,Q\xi) = \psi((QA)^*v,Q\xi) = \psi(A^*v,\xi),$$

so for any vectors $a, \xi \in \mathbb{R}^3$,

$$\psi(Qa,Q\xi) = \psi(a,\xi)$$
.

We claim that this implies that ψ is a function ψ_0 of the thre scalar quantities |a|, $a \cdot \xi$, and $|\xi|$. Indeed, we may suppose that $\xi = |\xi| e_1$. Then

$$a = (a^1, a^2, a^3) = \frac{a \cdot \xi}{|\xi|} e_1 + a^2 e_2 + a^3 e_3$$
.

Applying a suitable rotation P about the e1-axis gives

Pa =
$$\frac{a \cdot \xi}{|\xi|} e_1 + \{|a|^2 - (\frac{a \cdot \xi}{|\xi|})^2\}^{\frac{1}{2}} e_2$$

and

$$\psi(a,\xi) \ = \ \psi(Pa,P\xi) \ = \ \psi\Big(\frac{a\cdot\xi}{\mid\xi\mid}e_1 \ + \ \Big\{\mid a\mid^2 - \big(\frac{a\cdot\xi}{\mid\xi\mid}\big)^2\ \Big\}^{\frac{1}{2}}\ e_2, \mid \xi\mid e_1\ \Big).$$

This defines a function $\psi_o(\alpha,\beta,\gamma)$ such that

$$\psi(a,\xi) = \psi_0(|a|, a \cdot \xi, |\xi|)$$

and hence

$$\psi^{**}(A^*v,\xi) = \psi_{o}^{**}(|A^*v|, A^* \cdot \xi \otimes v, |\xi|). \tag{8.29}$$

It is easily checked that the rank- one convexity of $\tau^{\#}(A,\xi,\nu)$ implies that $\psi_o^{**}(\alpha,\beta,\gamma)$ is convex in (α,β) and increasing in α . QED

Appendix to section 8: proofs of the elementary facts

The group $\mathbb H$ is closed under transposition. Note that to show a. it is equivalent to show that there is a sequence $(H_\mu) \subset H$ such that

$$\frac{H_{\mu}e_1}{\mid H_{\mu}e_1\mid} \to \nu \qquad \text{as } \mu \to \infty \,.$$

Consider the two dimensional case first. Let $v \in S^1$ be given and write

$$\nu \ = \ \lim {}_{\mu \, \to \, \infty} \, \frac{1}{\sqrt{(h_{\mu}^1)^2 + (h_{\mu}^2)^2}} \, \, (h_{\mu}^1, \, h_{\mu}^2) \ , \label{eq:numbers}$$

where the (h^1_μ, h^2_μ) are integers. We may obviously assume that h^1_μ, h^2_μ are relatively prime, and thus, there are $p^1_\mu, p^2_\mu \in \mathbb{Z}$ such that

$$h_{\mu}^{1}p_{\mu}^{1} + h_{\mu}^{2}p_{\mu}^{2} = 1.$$

Let

$$H_{\mu} = \begin{pmatrix} h_{\mu}^{1} & -p_{\mu}^{2} \\ h_{\mu}^{2} & p_{\mu}^{1} \end{pmatrix}, \det H_{\mu} = 1,$$

so
$$H_{\mu}e_1 \ = \ h_{\mu} \ = \ \begin{pmatrix} h_{\mu}^1 \\ h_{\mu}^2 \end{pmatrix}$$

and (8.14) is satisfied.

Now identify H_{μ} with $H_{\mu} + e_3 \otimes e_3$ and $h \in \mathbb{R}^2$ with $(h,0) \in \mathbb{R}^3$. Note that if $k \in \mathbb{Z}$ and h^1 and h^2 are relatively prime with

$$h^1p^1 + h^2p^2 = 1$$
,

then

$$(1 + kp^1 e_3 \otimes e_3 + kp^2 e_3 \otimes e_3) h = h + k e_3.$$

Therefore it suffices to show that any $v \in \mathbb{S}^2$ may be written

$$\nu \ = \ \lim_{k \, \to \, \infty} \, \frac{1}{\sqrt{\mid h_{\mu} \mid^2 + (k_{\mu})^2}} \, \left(h_{\mu}^1, \, h_{\mu}^2, \, k_{\mu} \right) \, ,$$

where h_μ^1 , h_μ^2 are relatively prime. We may assume that $\nu^3>0$ and $\rho^2=(\nu^1)^2+(\nu^2)^2>0$. Let $h_\mu=(h_\mu^1,\,h_\mu^2,\,0)$ satisfy

$$\frac{h_{\mu}}{\mid h_{\mu}\mid} \rightarrow \frac{1}{\rho}(v^1, v^2, 0)$$
 as $\mu \rightarrow \infty$

with $\,h_{\mu}^1,\,h_{\mu}^2\,$ relatively prime. We may assume that $\,l\,h_{\mu}\,l\,\to\,\infty\,.$ Consider

$$v_{\mu} = \frac{1}{\sqrt{|h_{\mu}|^2 + (k_{\mu})^2}} (h_{\mu}^1, h_{\mu}^2, k_{\mu}),$$

$$k_{\mu} = \text{biggest integer in } \sqrt{\frac{1 - \rho^2}{\rho^2} |h_{\mu}|^2} + 1$$

 $= \sqrt{\frac{1-\rho^2}{\rho^2}|h_{\mu}|^2} + \epsilon_{\mu} \ , \quad 0 \leq \epsilon_{\mu} \leq 1.$

It is evident that $\,\nu_{\mu}\,\rightarrow\,\nu$.

Proof of b. This is an immediate consequence of the density of the rationals in the reals.

Proof of c. This is part of the standard twinning calculation. See Fonseca [16] for a more general fact. Suppose that

$$Q = \begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix}, \quad \alpha^2 + \beta^2 = 1,$$

and

$$A = 1 + \lambda e_1 \otimes e_2.$$

Then, if $\beta \neq 0$, Q – A has rank one for $\lambda = \frac{2(1-\alpha)}{\beta}$. Hence

$$Q = A (1 + a \otimes n) = \prod_{i=1}^{2} (1 + a_{i} \otimes n_{i})$$
 (8A.1)

is the product of two simple shears. If P = -1, choose Q above with $\beta \neq 0$. Consider

$$OP = -O$$
.

Then

$$-Q - A$$
 has rank one for $\lambda = -\frac{2(1+\alpha)}{\beta}$,

hence using (8A.1)

$$-1 = QA = \prod_{i=1}^{3} (1 + a_i \otimes n_i)$$
. QED

9 The minimum energy of the elastic crystal

In the examples of §7, the minimum value of E(u) was obtained as the sum of the separate minima of the bulk and surface terms. This is not true in general, as we should like to point out for the elastic crystal of §8. To estimate the minimum energy of the functional of (8.6), we shall impose the kinematical hypothesis that

$$\inf_{C} \mathcal{E}^{\#}(\mathbf{u}) = \inf_{C} \mathcal{E}^{\#}(\mathbf{u}), \qquad (9.1)$$

$$C = C^1(\overline{\Omega})$$
 and $C^+ = \{ u \in C^1(\overline{\Omega}) : \det \nabla u > 0 \}$.

This will be satisfied, for example, provided that ψ defined by (8.8) fulfills

$$\Psi(F^*v,\xi) = \inf_{A^*v = F^*v, \text{ det } A > 0} \tau(A,\xi,v).$$
 (9.2)

Recall that by the isoperimetric inequality, Federer [14], there is a constant $\,C_0>0\,$ such that

$$\left(\int\limits_{\Omega} \det \nabla v \ dx\right)^{\frac{2}{3}} \leq C_0 \int\limits_{\Gamma} |(\nabla v)^*v| \ dS \ , \qquad v \in C^1(\overline{\Omega}). \quad (9.3)$$

Let us consider a special case where

$$\Psi^{**} = g(|F^*v|), \qquad (9.4)$$

for example, $\psi^{**}(F^*v) = \gamma |F^*v|$ for a constant $\gamma > 0$. We may apply Jensen's inequality in this circumstance to each of the terms of the integral in (8.11). With $F = \nabla u$,

$$\int_{\Omega} \phi^{**}(\det F) dx \geq |\Omega| \phi^{**}\left(\frac{1}{|\Omega|}V\right),$$

$$V = \int_{\Omega} \det F \, dx$$

and

$$\int\limits_{\Gamma} g(\mid F^* v \mid) \, dx \ \geq \ [\Gamma] \ g(\frac{1}{[\Gamma]} \sigma) \, ,$$

$$\sigma = \int |F^*v| dS.$$

Adding these, we obtain

$$\mathcal{E}^{\#}(\mathbf{u}) \geq |\Omega| \phi^{**} \left(\frac{1}{|\Omega|} \mathbf{V}\right) + [\Gamma] g\left(\frac{|\Omega|^{2/3}}{C_0[\Gamma]} \mathbf{V}\right)$$
(9.5)

In general, the right hand side of (9.5) is larger than

$$|\Omega| \inf \phi^{**} + [\Gamma] \inf \psi^{**}$$
.

In case ψ^{**} also depends on $F^*v \cdot \xi$, for example, one may use the observation that

$$\int_{\Gamma} F^* \cdot u \otimes v \, dS = 3 \int_{\Omega} \det F \, dx = 3V.$$

Acknowledgements First of all, we wish to acknowledge E. De Giorgi whose suggestion led to our investigation of this question. We wish to thank J. L. Ericksen, I. Fonseca, R. Hardt, and R. James for their help and their interest. The second author also wishes to thank the I M A for its hospitality.

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