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Microstructures, phase transitions
and geometry

by

Stefan Müller

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Stefan Müller

Max-Planck-Institute for Mathematics in the Sciences

Inselstr. 22-26, 04103 Leipzig, Germany

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1 What are microstructures?

Microstructures are structures on a scale between the atomic scale and the macroscopic scale on which we usually make observations. They are abundant in natural and man-made materials, and often the microstructure optimizes a material's properties (maximum strength at given weight, minimal energy, maximum or minimum permeability, ...). Some materials can change their internal microstructure and hence their properties in response to external influences. They are sometimes referred to as 'smart materials' and are of great technological interest.

The attempt to mathematically describe and analyze the formation, interaction and the macroscopic effects of microstructures yields new, easily stated but deep mathematical problems. Their resolution is in its very beginning and involves the interaction of a variety of branches of mathematics including the calculus of variations, differential geometry, geometric measure theory, dynamical systems and nonlinear partial differential equations. In the following I try to describe some of the basic questions and how different branches of mathematics are involved in their resolution.

To simplify the exposition I focus on models of microstructures that arise in elastic crystals due to a solid-solid phase transformation. A large part of this article, in particular Sections 2-5, mainly reviews work of others. I draw heavily on the beautiful survey of Šverák [Sv 94] as well as the detailed expositions of Ball and James [BJ 87], [BJ 92]. Currently no exposition of the field in book form is available but various projects are in preparation [BJ 97a], [BJ 97b], [Mu 97a],[Mu 97b], [PZ 97]. Dacorogna's book [Da 89] is a good reference for the direct method and notions of convexity.

2 Microstructure in elastic crystals

Inspired by ideas of Ericksen, Ball and James [BJ 87] (see also [CK 88], [Fo 89]) proposed to study crystal microstructure by analyzing minimizers and minimizing sequences for the elastic energy. They use a continuum model based on nonlinear elasticity (a theory based on linearized elasticity was proposed earlier by Khachaturyan, Roitburd and Shatalov; see [Kh 67], [Kh 83], [KSh 69], [Ro 69], [Ro 78]; a comparison of the two approaches appears in [BJ 92], Section 9, [Bh 93] and [Ko 89]). The elastic energy I needed to deform the crystal from its reference configuration (identified with a bounded

domain $\Omega \subset \mathbf{R}^3$) by a map $u : \Omega \rightarrow \mathbf{R}^3$ is given by

$$I(u) = \int_{\Omega} W(Du)dx, \quad (2.1)$$

where $Du = (\frac{\partial u^i}{\partial x^j})$ is the deformation gradient. The Cauchy-Born rule asserts that the stored-energy density $W(F)$ is the energy (per unit reference volume) needed to perform an affine deformation $x \mapsto Fx$ of the crystal lattice. The stored energy is invariant under rigid transformations of the ambient space (frame indifference) and under changes of the independent variables that correspond lattice invariant rotations (crystal symmetry)

$$W(QF) = W(F) \quad \forall Q \in SO(3), \quad (2.2)$$

$$W(FR) = W(F) \quad \forall R \in \mathcal{P} \subset SO(3). \quad (2.3)$$

The discrete point group \mathcal{P} reflects the symmetry properties of the lattice that persist in the continuum approach (see [Er 80], [Er 89], [Pi 84] for the relevance of \mathcal{P} and [Er 84], [Za 92] for a discussion of the Cauchy-Born rule).

It is convenient to normalize W such that $\min W = 0$. Then the set

$$K = \{F : W(F) = 0\}$$

contains exactly the zero-energy affine deformations of the lattice. By (2.2) and (2.3) this set consists of one or several disjoint copies of $SO(3)$

$$K = SO(3)U_1 \cup \dots \cup SO(3)U_m, \quad U_i = U_i^T > 0. \quad (2.4)$$

In general the energy W and hence the set K depend on the temperature Θ . For materials that undergo solid-solid phase transitions K consists of one component at high temperatures and of several symmetry related (through \mathcal{P}) components below a critical temperature Θ_c (see [BJ 92]).

The relation between minimization of I and microstructure is discussed in Section 4 for a model problem; situations with $SO(n)$ symmetry are discussed in Section 5.

3 Basic mathematical questions

The fundamental problem is:

Characterize minimizers and minimizing

sequences of $I(u) = \int_{\Omega} W(Du)dx$
subject to suitable boundary conditions.

This is a very difficult problem since W is typically not convex (nor rank-1 convex) for materials that undergo solid-solid phase transitions. In other words the corresponding Euler-Lagrange equations are not strongly elliptic but of mixed elliptic-hyperbolic type. Research has therefore mostly focused on (almost) zero energy states, i.e. pointwise minimizers of the integrand. Generalizing the setting slightly we consider maps

$$u : \Omega \subset \mathbf{R}^n \rightarrow \mathbf{R}^m$$

on a bounded domain Ω (with Lipschitz boundary) and a compact set $K \subset M^{m \times n}$ in the $m \times n$ matrices (e.g. the zero set of W).

Problem 1 (exact solutions): Characterize all Lipschitz maps u such that

$$Du \in K \quad \text{a.e. in } \Omega. \quad (3.1)$$

Problem 2 (approximate solutions): Characterize all sequences u_j of maps whose Lipschitz constants are uniformly bounded and which satisfy

$$\text{dist}(Du_j, K) \rightarrow 0 \quad \text{a.e. in } \Omega. \quad (3.2)$$

Problem 3 (relaxation of K): Determine the sets K^{ex} and $K^{app} \subset M^{m \times n}$ of all matrices F such that Problem 1 and Problem 2 have a solution that satisfies in addition

$$u(x) = Fx \quad \text{on } \partial\Omega, \quad (3.3)$$

$$u_j(x) = Fx \quad \text{on } \partial\Omega, \quad (3.4)$$

respectively.

A simple covering and scaling argument shows that K^{ex} and K^{app} do not depend on Ω .

In the context of crystal microstructures the sets K^{ex} and K^{app} have an important interpretation. They represent *macroscopic* zero (or almost zero) energy deformations, while K represents *microscopic* zero energy deformations. The sets K^{ex} and K^{app} can be much larger than K ; in fact it is conjectured (and proved in two dimensions) that for many sets of the form

(2.4) the sets K^{ex} and K^{app} have interior points (subject to an incompressibility constraint $\det F = 1$). This would correspond to an (experimentally observed) fluid-like behavior. Some known results are reviewed in Section 5 below.

Problems 1-3 also arise in many other contexts, e.g. in the classification of isometric immersions or in the theory of nonlinear elliptic and hyperbolic partial differential equations, see Šverák's survey [Sv 94] and Gromov's treatise [Gr 86].

If minimizers do not exist there are often many different minimizing sequences. Some of those, however, only differ in rather superficial ways.

Problem 4: Develop mathematical objects that capture the 'essential features' of minimizing sequences.

One such object is the Young measure, discussed in Section 5; see also Section 8.1. Minimization of elastic energy often predicts minimizing sequences that develop finer and finer oscillations. Experimentally a limited fineness is observed.

Problem 5: Explain the length scale and fine geometry of microstructures, possibly by including other contributions to the energy, such as interfacial energy.

Some attempts in this directions are discussed in Section 7.

4 The two-gradient problem

Before reviewing a general framework for Problems 1-4 let us look at the simplest example

$$K = \{A, B\}.$$

4.1 Exact solutions

The simplest solution satisfies $Du = A$ on a halfspace H and $Du = B$ on its complement. Due to tangential continuity of u this is only possible if $B - A = a \otimes n$, where n is the normal to H . In particular one has $\text{rk}(B - A) = 1$. It turns out that for an arbitrary solution of $Du \in K$, the gradient can only jump across hyperplanes with normal n .

Lemma 4.1 ([BJ 87]). *Suppose that $u : \mathbf{R}^n \rightarrow \mathbf{R}^m$ is Lipschitz and*

$$Du \in \{A, B\} \text{ a.e.}$$

(i) *If $\text{rk}(B - A) > 1$ then $Du \equiv A$ a.e or $Du \equiv B$ a.e*

(ii) *If $\text{rk}(B - A) = 1$ then $B - A = a \otimes n$ and there exists a Lipschitz function $h : \mathbf{R} \rightarrow \mathbf{R}$ such that $h' \in \{0, 1\}$ a.e and*

$$u(x) = Ax + a h(x \cdot n).$$

The proof is a simple exercise using the fact that the distributional curl of a gradient vanishes.

4.2 Approximate solutions

Lemma 4.2 ([BJ 87]). *Suppose that $\text{rk}(B - A) > 1$ and let $u_j : \Omega \rightarrow \mathbf{R}^n$ be a sequence of functions with uniformly bounded Lipschitz constants that satisfy*

$$\text{dist}(Du_j, \{A, B\}) \rightarrow 0 \text{ a.e. in } \Omega.$$

Then (for a subsequence; not relabelled) either

$$Du_j \rightarrow A \text{ a.e. or } Du_j \rightarrow B \text{ a.e.}$$

This can be proved e.g. by using the minors relations (see Section 5).

4.3 Relaxation, nonattainment, microstructure

If $\text{rk}(B - A) > 1$ then $K^{app} = K$ by Lemma 4.2.

Lemma 4.3 ([BJ 87]). *Suppose that $\text{rk}(B - A) = 1$. Then*

(i) $K^{ex} = \{A, B\}$.

(ii) $K^{app} = \text{conv}K = \{\lambda A + (1 - \lambda)B : \lambda \in [0, 1]\}$.

Moreover for any sequence $u^{(j)}$ that satisfies (3.2) and (3.4) one has

$$u^{(j)} \rightarrow Fx \text{ uniformly on } \Omega. \tag{4.1}$$

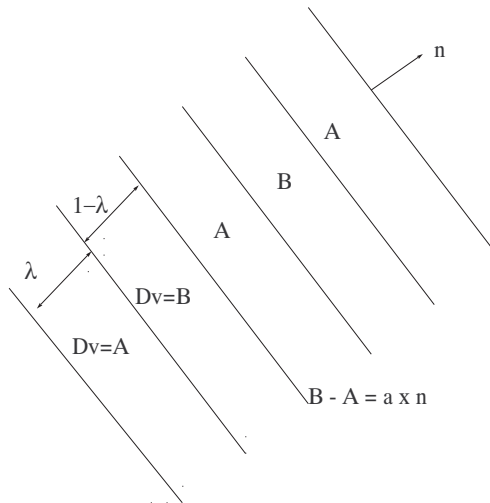


Figure 1: A simple laminate.

In particular for $\lambda \in (0, 1)$, $F = \lambda A + (1 - \lambda)B$ there exist approximate but not exact solutions. The gradients Du_j of minimizing sequences must oscillate rapidly so that u_j can approach Fx . Nonexistence of a minimizer thus leads to fine scale oscillations and ‘microstructure’.

We sketch one possible construction of a minimizing sequence. Many variants are possible, and we return in Section 5 to the question whether all minimizing sequences are unique up to minor details.

Assume without loss of generality that $F = 0$, let h be a 1-periodic Lipschitz function with $h' = -(1 - \lambda)$ on $(0, \lambda)$, $h' = \lambda$ on $(\lambda, 1)$ and let

$$v(x) = h(x \cdot n), \quad v_k(x) = k^{-1}v(kx).$$

The functions v_k are called simple laminates since the sets $\{Du = A\}$ and $\{Du = B\}$ consist of parallel stripes (see Figure 1). We have $Dv_k \in \{A, B\}$ a.e and $v_k \rightarrow 0$ uniformly. To adjust the boundary conditions consider the cut-off functions $\varphi_k(x) = \min\{k \text{dist}(x, \partial\Omega), 1\}$. Then $u_k = \varphi_k v_k$ has the desired properties.

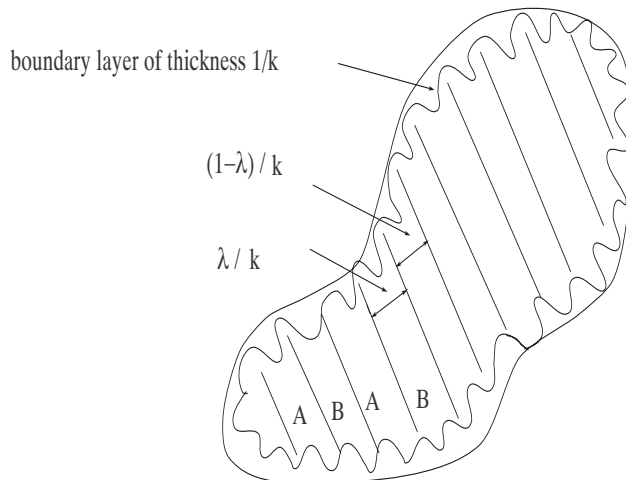


Figure 2: A minimizing sequence obtained by truncation of very fine laminates.

5 Approximate solutions and Young measures

Young measures (also called ‘generalized functions’) were introduced by L.C. Young in the 30’s to solve optimal control problems that have no classical solution but rather require an infinitesimally fast switching between states (see [Yo 37], [Yo 69]). The idea is to replace functions which take values in a (compact) set K by functions that take values in the space of probability measures on K . Thus an ‘infinitesimally fine’ mixture of two states is represented by a convex combination of two Dirac masses. For the problems discussed above it is crucial to characterize those Young measures that are generated by sequences of gradients. An abstract characterization is available in terms of quasiconvex functions, but already simple concrete examples lead to challenging open questions, since very few quasiconvex functions are known.

The presentation below follows [Ba 89]. A short selection of the rich literature on Young measures is [Ba 84], [BL 73], [Kr 94], [Va 90], [Va 94]. Tartar [Ta 79], [Ta 82] and later DiPerna [DP 85] used Young measures in connection with the theory of compensated compactness to analyze compactness and existence questions in nonlinear partial differential equations. Varifolds

([Al 72]) are a generalization of Young measures to a geometric setting.

Let E be a measurable set in \mathbf{R}^n , K a compact set in \mathbf{R}^l and denote by $\mathcal{M}(K)$ and $\mathcal{P}(K)$ the space of the Radon measures and of probability measures on K . The pairing between the space $C(K)$ of continuous functions and its dual $\mathcal{M}(K)$ is denoted by $\langle \mu, f \rangle = \int_K f d\mu$. A *Young measure* $\nu : E \rightarrow \mathcal{P}(K)$ is a weak* measurable map, i.e. a map such that $x \mapsto \langle \nu(x), f \rangle$ is measurable for all $f \in C(K)$.

Theorem 5.1 (*Fundamental theorem on Young measures*)

Let $w_j : E \rightarrow K$ be a sequence of measurable functions. Then there exists a subsequence w_{j_k} and a Young measure $\nu : E \rightarrow \mathcal{P}(K)$ such that for all $f \in C(K)$

$$f(w_{j_k}) \xrightarrow{*} f_\infty \text{ in } L^\infty(E), \quad f_\infty(x) = \langle \nu_x, f \rangle = \int_K f d\nu_x. \quad (5.1)$$

Moreover if $K' \subset K$ is a compact subset then:

$$\text{supp} \nu_x \subset K' \text{ for a.e. } x \iff \text{dist}(w_{j_k}, K') \rightarrow 0 \text{ (locally) in measure.} \quad (5.2)$$

Notation: We say that the sequence w_{j_k} generates the Young measure ν . A Young measure ν is called a $(W^{1,\infty})$ -gradient Young measure if E is open and there exists a sequence u_j Lipschitz functions with uniformly bounded Lipschitz constants such that Du_j generates ν .

Remark. A similar result holds for sequences $w_j : E \rightarrow \mathbf{R}^l$ if one replaces $C(K)$ by $C_0(\mathbf{R}^l)$, the dual of $\mathcal{M}(\mathbf{R}^l)$. In this case, however, $\nu(x)$ is in general only a subprobability measure. Mild additional condition such as $\sup_j \int_E |w_j|^s < \infty$ for some $s > 0$ assure that $\nu(x)$ is a probability measure.

Alternatively one can work in a suitable compactification of \mathbf{R}^l .

Proof. To each w_j we associate the elementary Young measure

$$\nu_j(x) = \delta_{w_j(x)}.$$

The sequence $\{\nu_j\}_{j \in \mathbf{N}}$ is bounded in the space $L_w^\infty(E; \mathcal{M}(K))$ of essentially bounded, weak* measurable maps. Since this space is a dual of $L^1(E; C(K))$ (see [Ed 65], p. 588; [IT 69], p. 93; [Me 66], p. 244) the first assertion follows from the Banach-Alaoglu theorem and the fact that $\mathcal{P}(K)$ is weak* closed in $\mathcal{M}(K)$. The second assertion is a simple consequence of the first. \square

Young measures are closely related to compactness by the following fact.

Corollary 5.2 *Let w_{j_k} be as in Theorem 5.1. Then*

$$w_{j_k} \rightarrow w \text{ locally in measure} \iff \nu(x) = \delta_{w(x)} \quad \text{a.e.}$$

Young measures provide a concise description of the fine scale oscillation that may arise in minimizing sequences.

Example 5.3 As in Section 4.3 consider $A, B, F \in M^{m \times n}$ with $\text{rk}(B - A) = 1$, $F = \lambda A + (1 - \lambda)B$, $\lambda \in (0, 1)$. Let u_j be a sequence with $\text{dist}(Du_j, \{A, B\}) \rightarrow 0$ a.e., $u_j(x) = Fx$ on $\partial\Omega$. Then Du_j generates the (unique) Young measure $\lambda\delta_A + (1 - \lambda)\delta_B$.

Proof. By (5.2), $\text{supp } \nu(x) \subset \{A, B\}$. Hence $\nu(x) = \mu(x)\delta_A + (1 - \mu(x))\delta_B$. Application of (5.1) with $f = \text{id}$ and Lemma 4.3 (ii) yield $\mu(x)A + (1 - \mu(x))B = F$, which implies the assertion. \square

Young measures can be seen as generalized solutions of the problem $Du \in K$ or $\int_{\Omega} W(Du) \xrightarrow{!} \min$ generated by minimizing sequences. A classical solution corresponds to a Young measure that is a Dirac mass at every point. Problem 2 (approximate solutions) can be rephrased as follows.

Problem 2': Characterize all gradient Young measures supported in K .

To classify gradient Young measures Morrey's notion of quasiconvexity is fundamental.

Definition 5.4 *A function $f : M^{m \times n} \rightarrow \mathbf{R}$ is quasiconvex if for every bounded domain Ω and every $F \in M^{m \times n}$*

$$\int_{\Omega} f(F + D\varphi) \geq \int_{\Omega} f(F) = |\Omega|f(F), \quad \forall \varphi \text{ Lipschitz}, \varphi|_{\partial\Omega} = 0. \quad (5.3)$$

Thus f is quasiconvex if affine functions minimize $\int_{\Omega} f(Du)$ subject to affine boundary values. The definition is independent of Ω , and quasiconvex functions are automatically continuous.

Morrey's crucial observation was that quasiconvexity of f is equivalent to (sequential) $W^{1, \infty}$ weak* lower semicontinuity of the functional $u \mapsto \int_{\Omega} f(Du)dx$. Combining this fact with careful measure-theoretic and functional-analytic arguments, Kinderlehrer and Pedregal obtained the following classification.

Theorem 5.5 ([KP 91]) *A Young measure $\nu : \Omega \rightarrow \mathcal{P}(M^{m \times n})$ is a $(W^{1,\infty}$ -) gradient Young measure if and only if the following three conditions hold*

- (i) *supp ν_x is uniformly bounded (for a.e. x);*
- (ii) *$\langle \nu_x, \text{id} \rangle$ is the gradient of a Lipschitz function;*
- (iii) *$f(\langle \nu_x, \text{id} \rangle) \leq \langle \nu_x, f \rangle$ for all quasiconvex f .*

The key point is (iii) which is in nice duality with Definition 5.4. Roughly speaking, quasiconvex function satisfy Jensen's inequality for gradients while gradient Young measures must satisfy Jensen's inequality for all quasiconvex functions. A similar result holds for Young measures generated by gradients of sequences that are bounded in the Sobolev space $W^{1,p}$ ($p > 1$), see [KP 94], [Kr 94], [FMP 97]; general references on Young measures for noncompact targets include [DPM 87] and [Ro 96].

As a consequence we obtain an abstract solution of Problem 2' and Problem 3. A Young measure ν is called homogeneous if the map $x \mapsto \nu(x)$ is constant (a.e.). A blow-up argument shows that if ν is a gradient Young measure then $\nu(a)$ arises as a homogeneous gradient Young measure for a.e. $a \in \Omega$, see [KP 91].

Corollary 5.6 *Let $K \subset M^{m \times n}$ be compact.*

- (i) *The set of homogeneous gradient Young measures supported on K is given by*

$$\mathcal{M}^{qc}(K) := \{\nu \in \mathcal{P}(K) : f(\langle \nu, \text{id} \rangle) \leq \langle \nu, f \rangle \quad \forall f : M^{m \times n} \rightarrow \mathbf{R} \text{ quasiconvex}\}.$$

- (ii) *The set K^{app} is the quasiconvex hull of K ,*

$$\begin{aligned} K^{app} &= K^{qc} := \{F : f(F) \leq \inf_K f, \quad \forall f : M^{m \times n} \rightarrow \mathbf{R} \text{ quasiconvex}\} \\ &= \{\langle \nu, \text{id} \rangle : \nu \in \mathcal{M}^{qc}(K)\}. \end{aligned}$$

Following Šverák we say that $\mathcal{M}^{qc}(K)$ is trivial if it only contains Dirac masses. In view of Corollary 5.2 this occurs if and only if all approximating sequences are compact.

Quasiconvexity is a natural condition, but hard to verify. Therefore two algebraic conditions were introduced. A function $f : M^{m \times n} \rightarrow \mathbf{R}$ is *polyconvex*

if it can be expressed as a convex function of minors (subdeterminants); it is called *rank-1-convex* if it is convex on all line segments $[A, B]$ with $\text{rank } B - A = 1$. One has the implications ([Mo 52]; [Da 89]).

$$f \text{ polyconvex} \Rightarrow f \text{ quasiconvex} \Rightarrow f \text{ rank-1 convex.}$$

For $m = 1$ or $n = 1$ all notions are equivalent to ordinary convexity. For $m, n \geq 2$ quasiconvexity does not imply polyconvexity.

Conjecture 5.7 (*Morrey, 1952*). *For $m, n \geq 2$ rank-1 convexity does not imply quasiconvexity.*

Šverák [Sv 92a] proved the conjecture for $m \geq 3$. The case $m = 2$ is open. Kristensen [Kr 97] very recently proved that for $m \geq 3$ there is no local condition that implies quasiconvexity.

For a minor M application of Theorem 5.5 to $\pm M$ yields the minors relation

$$\langle \nu_x, M \rangle = M(\langle \nu_x, \text{id} \rangle) \tag{5.4}$$

as a necessary condition for gradient Young measures. The following table illustrates some solved and unsolved problems for homogeneous gradient Young measures.

K	Nontrivial exact soln.	Nontrivial GYM	Method	References
$\{A, B\}$	No	No	Minors or Cauchy-Riemann eqns.	[BJ 87] [Sv 91a]
$\{A, B, C\}$	No	No	Nonconvex solns. of Monge-Ampère	[Sv 91b] [Sv 92b]
finite	?	Yes	Example with four matrices	[AH 86], [Ta 93], [CT 93], [BFJK 94]
countable	Yes	Yes	Example	[Sv]
$SO(2); \mathbf{R}SO(2)$	No;	No	Cauchy-Riemann eqns.	[Sv 91a]
$SO(n); \mathbf{R}SO(n)$	holomorphic fns.	No	Minors;degenerate elliptic eqns.	[Ki 88] [Re 68]
$n \geq 3$	No;	No	Minors or elliptic regularity	[Sv 93]
$\cup_{i=1}^k SO(2)A_i$	No	No	Special cases known	[Ma 93], [Sv 93]
$SO(3)A \cup SO(3)B$?	?	compensated compactness;	[Ta 79]
scalar conservation laws	No	No	div-curl lemma	
$m \times 2$ elliptic systems	?	Yes, $m \geq 6$?, $m < 6$		[Sv 94]

Table 1: Nontrivial exact solutions and nontrivial gradient Young measures (GYM) of incompatible sets K (i.e. $\text{rk}(A - B) \neq 1 \forall A, B \in K$); see [Sv 94], [BFJK 94] and the references therein for further examples.

6 Exact solutions and convex integration

Approximate solutions are characterized by the quasiconvex hull K^{qc} and set $\mathcal{M}^{qc}(K)$ of Young measures. The construction of exact solutions is more delicate. In view of the negative result for the two-gradient problem (see Lemma 4.3 (i)) it was widely believed that exact solutions are rather rare. Recent results suggest that many exact solutions exist but that they have to be very complicated. This is reminiscent of rigidity and flexibility results on isometric immersions and other geometric problems (see [Na 54]; [Ku 55]; [Gr 86], Section 2.4.12).

To illustrate some of the difficulties consider the two-dimensional two-well problem:

$$Du \in K \text{ a.e. in } \Omega, \quad u = Fx \text{ on } \partial\Omega, \quad (6.1)$$

$$K = SO(2)A \cup SO(2)B, \quad (6.2)$$

$$A = \text{Id}, \quad B = \text{diag}(\lambda, \mu), \quad 0 < \lambda < 1 < \mu. \quad (6.3)$$

If we ignore boundary conditions the simplest solutions of $Du \in K$ are simple laminates, see Figure 1. A short analysis of the rank-1 connections in K shows that such laminates are perpendicular to one of the normals n_1 or n_2 , determined by the two solutions of the equation

$$QA - B = a \otimes n. \quad (6.4)$$

There is, however, no obvious way to combine the two laminates (see Figure 4). It was thus believed that the problem (6.1) – (6.3) has no nontrivial solutions. This is false. The construction of nontrivial solutions is based on Gromov's method of convex integration.

6.1 Existence of solutions

First, one observes that the open version of the two-gradient problem admits a solution.

Lemma 6.1 ([MS 96]). *Suppose that $\text{rk}(B - A) = 1$, $F = \lambda A + (1 - \lambda)B$, $\lambda \in (0, 1)$. Then, for a bounded domain Ω and every $\epsilon > 0$ there exists a piecewise*

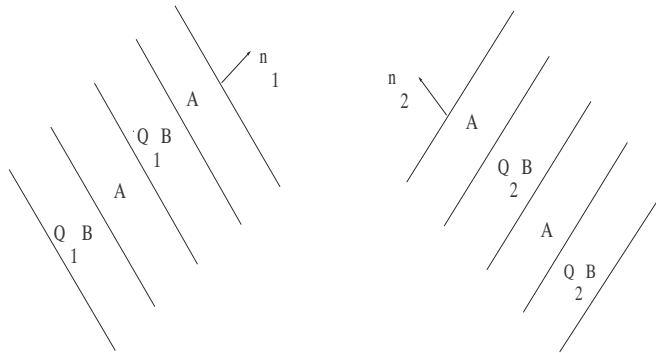


Figure 3: Two possible laminates for the two-well problem.

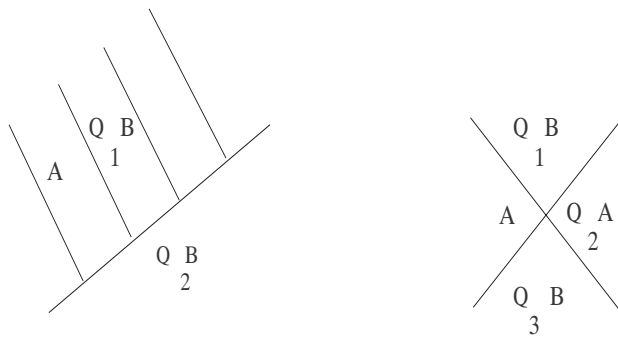


Figure 4: None of the above constructions satisfies the rank-1 condition across every interface.

linear map u such that

$$\begin{aligned} u(x) &= Fx \text{ on } \partial\Omega \\ \text{dist}(Du, \{A, B\}) &< \epsilon, \\ \sup |u(x) - Fx| &< \epsilon. \end{aligned}$$

Here a map $u : \Omega \rightarrow \mathbf{R}^m$ is called piecewise linear if u is Lipschitz continuous and if there exist finite or countably many disjoint open sets Ω_i whose union has full measure such that $u|_{\Omega_i}$ is affine. To iterate the result of Lemma 6.1 we define the lamination convex hull K^l of a set $K \subset M^{m \times n}$ by successive addition of rank-1 segments:

$$\begin{aligned} K^0 &:= K, \\ K^{(i+1)} &:= K^{(i)} \cup \{\lambda A + (1 - \lambda)B, \lambda \in (0, 1), A, B \in K^{(i)}, \text{rk}(B - A) = 1\} \\ K^l &:= \bigcup_{i=1}^{\infty} K^{(i)}. \end{aligned}$$

Remark. In contrast with the ordinary convex hull there is no version of Carathéodory's theorem that guarantees that the union of a fixed number of the $K^{(i)}$ is sufficient. Generally, very little is known about the geometry of rank-1 convexity (but see [MP 96]).

Lemma 6.2 *Suppose that $U \subset M^{m \times n}$ is open. Let $v : \Omega \rightarrow \mathbf{R}^m$ be piecewise affine and Lipschitz continuous and suppose $Dv \in U^l$ a.e. Then there exist $u : \Omega \rightarrow \mathbf{R}^m$ such that*

$$Du \in U \text{ a.e. in } \Omega, \quad u = v \text{ on } \partial\Omega.$$

The crucial step is the passage from open to compact sets $K \subset M^{m \times n}$. Following Gromov we say that a sequence of sets U_i is an in-approximation of K if

- (i) the U_i are open and contained in a fixed ball
- (ii) $U_i \subset U_{i+1}^l$
- (iii) $U_i \rightarrow K$ in the following sense: if $F_{i_k} \in U_{i_k}, i_k \rightarrow \infty$ and $F_{i_k} \rightarrow F$, then $F \in K$.

Theorem 6.3 ([Gr 86], p. 218; [MS 96]). *Suppose that K admits an in-approximation $\{U_i\}$. Let $v \in C^1(\Omega, \mathbf{R}^m)$ with*

$$Dv \in U_1.$$

Then there exists a Lipschitz map u such that

$$Du \in K \in \Omega \text{ a.e., } u = v \text{ on } \partial\Omega.$$

The proof uses a sequence of approximations obtained by successive application of Lemma 6.2. To achieve strong convergence each approximation uses a much finer spatial scale than the previous one, similar to the construction of continuous but nowhere differentiable functions. This is one of the key ideas of convex integration.

This theorem applies to the two-well problem (6.1) – (6.3) if $\lambda\mu \neq 1$. A calculation shows that solutions exist if $F \in \text{int } K^l$, and K^l is given by a simple formula (see [Sv 93]). A different construction of (many) nontrivial solutions was recently obtained by Dacorogna and Marcellini [DM 96b] using Baire’s theorem. Other existence results appear in [DM 96a], [DM 97]. The case $\lambda\mu = 1$ in (6.1) – (6.3) requires (i) of the following refinement.

Theorem 6.4 ([MS 97]). *Theorem 6.3 remains valid if the definition of in-approximation is modified as follows.*

- (i) *the sets U_i are relatively open in the set $\{F \in M^{n \times n} : \det F = 1\}$, $n > 1$.*
- (ii) *the lamination convex hull U^l is replaced by the rank-1 convex hull*

$$U^{rc} := \left\{ F \in M^{m \times n} : f(F) \leq \inf_U f \text{ for} \right. \\ \left. \text{all rank-1 convex } f : M^{m \times n} \rightarrow \mathbf{R} \right\}.$$

Part (i) just requires only a modification in the proof of Lemma 6.1. A completely open problem is how many constraints on F can be prescribed. A natural guess is that all minors can be prescribed but this is false.

Regarding part (ii) one trivially has the inclusion $K^l \subset K^{rc}$. Several authors ([AH 86], [CT 93], [Ta 93]) discovered independently an example where $K^{rl} \neq K^{rc}$. Let

$$K = \left\{ \pm \begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}, \pm \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix} \right\}$$

one has $K^l = K$ but

$$K^{rc} \supset \left\{ \begin{pmatrix} \lambda & 0 \\ 0 & \mu \end{pmatrix} : |\lambda| \leq 1, |\mu| \leq 1 \right\}.$$

It follows from Theorem 6.4 (ii) that the relation $Du \in U$ admits nontrivial solutions for every (small) neighbourhood U of K , although U contains no rank-1 connections (i.e. no simple laminates solve the relation).

A natural question is whether one can use the quasiconvex hull U^{qc} instead of U^{rc} . One key point seems to be the resolution of the following.

Conjecture 6.5 *Let K be a compact quasiconvex set, i.e. $K^{qc} = K$ and let $\nu \in \mathcal{M}^{qc}(K)$. Then for every open set $U \supset K$ there exists a sequence $u_j : (0, 1)^n \rightarrow \mathbf{R}^m$ such that Du_j generates ν and $Du_j \in U$ a.e.*

The conjecture is true for compact convex sets ([Mu 97a]); this refines a result of Zhang [Zh 92] who showed that $Du_j \in B(0, R)$ for a sufficiently large ball.

The use of the rank-1 convex hull U^{rc} rather than U^l is potentially relevant for the construction of singular solutions to $m \times 2$ elliptic systems

$$\operatorname{div} \sigma(Dv) = 0, \quad v : \Omega \subset \mathbf{R}^2 \rightarrow \mathbf{R}^m.$$

Such a system may be written as first order system (see [Sv 94])

$$Du \in K := \{(F, G) \in M^{2m \times 2}, \sigma(F) = G^\perp\},$$

where $G_{i1}^\perp = -G_{i2}$, $G_{i2}^\perp = G_{i1}$. Ellipticity implies that $K^l = K$, but nontrivial solutions may exist if one can show $K^{rc} \neq K$.

6.2 Regularity and rigidity

The construction outlined above yields very complicated solutions of the two-well problem (6.1) – (6.3). This raises the question whether the geometry of the solutions can be controlled. Consider the set

$$E = \{x \in \Omega : Du(x) \in SO(2)A\}$$

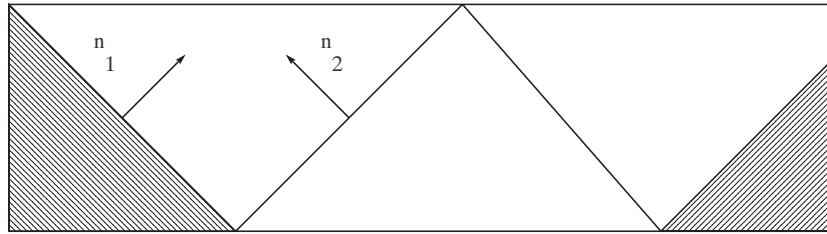


Figure 5: Structure of solutions with finite perimeter. The normals n_1, n_2 are determined by (6.4).

where Du takes values in one connected component of K (or one phase in the applications to crystals). The perimeter of a set $E \subset \Omega \subset \mathbf{R}^n$ is defined as

$$\text{Per}E = \sup_E \left\{ \int \text{div } \varphi \, dx : \varphi \in C_0^1(\Omega, \mathbf{R}^n), |\varphi| \leq 1 \right\}.$$

For smooth or polyhedral sets this agrees with the $(n - 1)$ dimensional measure of ∂E .

Theorem 6.6 ([DM 95]). *If u is a solution of (6.1) - (6.3) and if $\text{Per}E < \infty$ then u is locally a simple laminate and ∂E consists of straight line segments that can only intersect at $\partial\Omega$.*

The proof combines geometric and measure-theoretic ideas. The geometric idea is that the Gauss curvature $K(g)$ of the pull-back metric $g = (Du)^T Du$ should vanish (in a suitable sense). Since g only takes two values this should give information on E .

To implement this idea one first establishes a version of Liouville's theorem (infinitesimal rotations on an open connected set are rigid motions) for sets of finite perimeter. The analogue of connected components in this frame work are indecomposable components (a set F of finite perimeter is indecomposable if for every $F_1 \subset F$ with $\text{Per}F = \text{Per}F_1 + \text{Per}(F \setminus F_1)$ the set F_1 or $F \setminus F_1$ has zero measure). To finish the proof one decomposes Du as $e^{i\Theta} g^{1/2}$ (with the usual identification $\mathbf{C} \simeq \mathbf{R}^2$) and analyzes the jump conditions at the boundary of each component to deduce that Θ takes only two values and solves (in the distributional sense) a wave equation with characteristics n_1

and n_2 . Using more subtle arguments Kirchheim [Ki 97] has recently proved a similar rigidity result for

$$K = SO(3)U_1 \cup SO(3)U_2 \cup SO(3)U_3$$

where $U_1 = \text{diag}(\lambda, \mu, \mu)$ and U_2, U_3 are obtained by permuting the entries. An important additional difficulty is that $SO(3)$ is not abelian and one can thus not derive a linear equation for a suitable lift like Θ in the two-dimensional case.

7 Length scales, surface energy and singular perturbations

Minimization of elastic energy does not determine the length scale of the microstructure. If the infimum of the energy is not attained, minimizing sequences develop increasingly finer oscillations and generalized Young measure solutions correspond to an ‘infinitely fine’ microstructure. Also the Young measure only records the asymptotic volume fraction of each phase but not their geometric arrangement.

It is believed that addition of small surface (or higher gradient) energy contribution can remedy these deficiencies. The precise form of the surface energy term is not obvious. Popular choices for the total energy are

$$I^\epsilon(u) = \int_{\Omega} W(Du) + \epsilon^2 |D^2 u|^2 dx$$

or

$$I^\epsilon(u) = \int_{\Omega} W(Du) dx + \int_{\Omega} \epsilon |D^2 u|,$$

where $|D^2 u|$ is understood as a Radon measure. The idea is to study minimizers of these functional in the limit $\epsilon \rightarrow 0$. Almost nothing is known about the three-dimensional model with full $SO(3)$ symmetry but results on lower dimensional models already show very interesting behaviour.

7.1 A one dimensional model

As a caricature of the two-gradient problem consider

$$I(u) = \int_0^1 (u_x^2 - 1)^2 + u^2 dx \xrightarrow{!} \min \quad (7.1)$$

subject to periodic boundary conditions. Clearly $I(u) > 0$ since the conditions $u = 0$ a.e. and $u_x = \pm 1$ a.e. are incompatible. On the other hand $\inf I = 0$, since a sequence of finely oscillating sawtooth functions u_j can achieve $u_{jx} \in \{\pm 1\}$, $u_j \rightarrow 0$ uniformly. For any such sequence u_{jx} generates the (unique) Young measure $\nu = \frac{1}{2}\delta_{-1} + \frac{1}{2}\delta_1$. Note that there are many ‘different’ sequences that generate this Young measure.

Minimizers of the singularly perturbed functional

$$I^\epsilon(u) = \int_0^1 \epsilon^2 u_{xx}^2 + (u_x^2 - 1)^2 + u^2 dx$$

yield a very special minimizing sequence for I .

Theorem 7.1 ([Mu 93]). *If $\epsilon > 0$ is sufficiently small then every minimizer of I^ϵ (subject to periodic boundary conditions) is periodic with minimal period $P^\epsilon = 4(2\epsilon)^{1/3} + \mathcal{O}(\epsilon^{2/3})$.*

7.2 Surface energy and domain branching

Consider the two-dimensional scalar model problem (see [KM 92] for the relation with three-dimensional elasticity)

$$I(u) = \int_0^1 \int_0^L u_x^2 + (u_y^2 - 1)^2 dx dy \xrightarrow{!} \min$$

$$u = 0 \text{ on } x = 0. \quad (7.2)$$

The integrand is minimized at $Du = (u_x, u_y) = (0, \pm 1)$. The preferred gradients are incompatible with the boundary condition. The infimum of I subject to (7.2) is zero but not attained. The gradients Du_j of any minimizing sequence generate the Young measure $\frac{1}{2}\delta_{(0,-1)} + \frac{1}{2}\delta_{(0,1)}$. One possible construction of a minimizing sequence is as follows (see Figure 6). Let s_h be a periodic sawtooth function with period h and slope ± 1 and let $u(x, y) = s_h(y)$ for $x \geq \delta$, $u(x, y) = \frac{x}{\delta}s_h(y)$ for $0 \leq x < \delta$. Then consider a limit $h \rightarrow 0, \delta \rightarrow 0$ such that h/δ remains bounded. Similar reasoning applies if we replace (7.2)

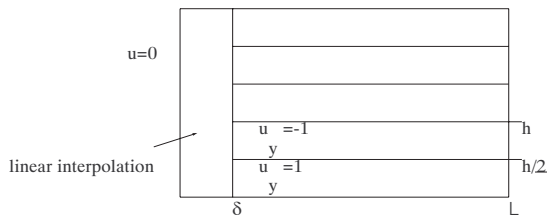


Figure 6: Construction of a minimizing sequence.

by the condition that u vanishes on the whole boundary of $[0, L] \times [0, 1]$.

To understand the influence of regularizing terms on the length scale and the geometry of the fine scale structure we consider

$$I^\epsilon(u) = \int_0^1 \int_0^L u_x^2 + (u_y^2 - 1)^2 + \epsilon^2 u_{yy}^2 dx dy,$$

subject to (7.2). Instead of the second derivatives in y one can consider other regularizing terms, e.g. $|D^2 u|^2$. The derivatives in y are, however, the most important ones, since we expect that fine scale oscillations arise mainly in the y direction. It was widely believed that for small $\epsilon > 0$ the minimizers of I^ϵ look roughly like the construction $u_{h,\delta}$ depicted in Figure 6 (with the corners of the sawtooth ‘rounded off’ and optimal choices $\delta(\epsilon), h(\epsilon)$). This is false. Indeed a short calculation shows that $\delta(\epsilon) \sim (\epsilon L)^{1/2}$, $h(\epsilon) \sim (\epsilon L)^{1/2}$ and $I^\epsilon(u_{h,L}^\epsilon) \sim \epsilon^{1/2} L^{1/2}$. On the other hand one has

Theorem 7.2 ([Sch 94]). *For $0 < \epsilon < 1$ there exists constants $c, C > 0$ such that*

$$c\epsilon^{2/3} L^{1/3} \leq \min_{u=0 \text{ at } x=0} I^\epsilon \leq C\epsilon^{2/3} L^{1/3}.$$

The upper bound is obtained by a smooth version of the self-similar construction depicted in Figure 7.

The mathematical issues become clearer if we replace I^ϵ by a sharp interface version

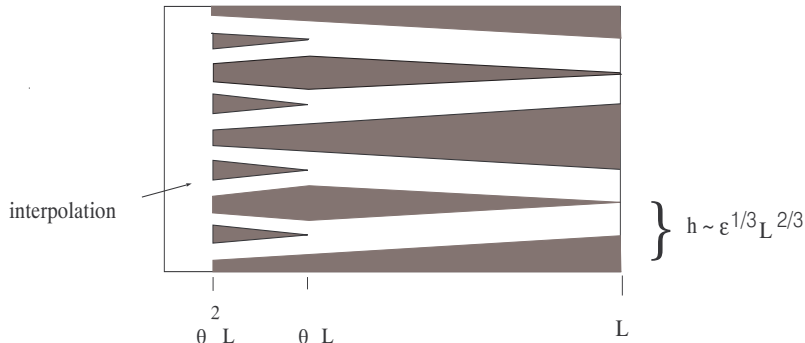


Figure 7: The self-similar construction with $1/4 < \Theta < 1/2$. Only two generations of refinement are shown.

$$J^\epsilon(u) = \int_0^L \int_0^1 u_x^2 + \epsilon |u_{yy}| dy dx \quad (7.3)$$

subject to

$$|u_y| = 1 \text{ a.e.} \quad (7.4)$$

Thus $y \mapsto u(x, y)$ is a sawtooth function and $\int_0^1 |u_{yy}| dy$ denotes twice the number of jumps of u_y . Minimization of (7.3) subject to (7.4) is in fact a purely geometric problem for the set

$$E = \{(x, y) : u_y(x, y) = 1\}.$$

The first term in J^ϵ is a nonlocal energy in terms of E , while the second is essentially the length of ∂E (more precisely its projection to the x -axis; as before we consider this to be the essential part since oscillations occur mainly in the y direction). The functional and the constraint are invariant under the scaling

$$u_\lambda(x, y) = \lambda^{-1} u(\lambda^{3/2} x, \lambda y)$$

which suggests a self-similar construction with $\Theta = (\frac{1}{2})^{3/2}$.

Theorem 7.3 ([KM 94]). For $0 < \epsilon < 1$

$$c\epsilon^{2/3} L^{1/3} \leq \min_{(7.3)(7.4)} J^\epsilon \leq C\epsilon^{2/3} L^{1/3}.$$

Moreover if \bar{u} is a minimizer of J^ϵ subject to (7.3), (7.4) then

$$c\epsilon^{2/3}l^{1/3} \leq \int_0^1 \int_0^l \bar{u}_x^2 + \epsilon|\bar{u}_{yy}| \leq C\epsilon^{2/3}l^{1/3}. \quad (7.5)$$

The scaling in (7.5) is exactly the scaling predicted by the self-similar construction with $\theta = (\frac{1}{2})^{3/2}$.

Conjecture 7.4 *As $\epsilon \rightarrow 0, l \rightarrow 0$ the rescaled minimizers*

$$v_\epsilon(x, y) = \epsilon^{-1/3}l^{-2/3}\bar{u}_\epsilon(lx, \epsilon^{1/3}l^{2/3}y)$$

converge to a self-similar function (at least for a subsequence).

The prediction of refinement of the microstructure (domain branching) towards the boundary $x = 0$ in the simple models (7.3), (7.4) inspired new experimental investigations ([Sch 93]). In closely related models for magnetization domains in ferromagnetic materials domain branching is experimentally well established ([Li 44], [Hu 67], [Pr 76]), a rigorous mathematical analysis is just beginning to emerge. Already a quick look at some of the sophisticated constructions in [Pr 76] suggests that a lot is to be discovered.

8 Outlook

To close I briefly mention three questions in the analysis of microstructures that are widely open:

- Which mathematical object describes microstructure most efficiently?
- What is the rôle of dynamics?
- How can one efficiently compute microstructures?

8.1 Beyond Young measures

Young measures are but one way to extract ‘relevant’ information from a rapidly oscillating sequence. They describe the asymptotic local phase proportions in a finer and finer mixture. The Young measure contains no information about the geometry of the mixture, self correlations of the sequence or relevant length scales.

There is an intense search for new objects that record more information, and Tartar’s article [Ta 95], from which the title of this subsection was borrowed, gives a recent survey. Due to space constraints I can only briefly

mention two such objects: the H -measure and its variants which already found many applications and the two-scale Young measure which still has to prove its usefulness.

A typical example where knowledge of local phase proportions is insufficient arises in the theory of homogenization. A fine laminate of a good and a poor heat conductor behaves macroscopically like an anisotropic material that conducts poorly in the direction of lamination and well in the perpendicular directions.

To take the influence of the layering direction into account Tartar [Ta 90] introduced the H -measure that acts simultaneously on real space and on Fourier space. The same object was introduced independently by Gérard [Ge 91] under the name ‘microlocal defect measure’. For every sequence $u_j \rightharpoonup 0$ $L^2(\Omega)$ there exists a subsequence u_{j_k} and a Radon measure μ on $\bar{\Omega} \times S^{n-1}$ (the H -measure of $\{u_{j_k}\}$) such that for every pseudo-differential operator A of order zero with (sufficiently regular) symbol $a(x, \xi)$ one has

$$\langle Au_{j_k}, u_{j_k} \rangle_{L^2} \rightarrow \int_{\bar{\Omega} \times S^{n-1}} ad\mu.$$

For \mathbf{R}^m -valued sequences one similarly obtains a matrix-valued (hermitian) measure $\nu = (\nu^{ij})_{1 \leq i, j \leq m}$. Applications of H -measures include small amplitude homogenization, compensated compactness with variable coefficients, compactness by averaging in kinetic equations and the propagation of energy concentrations in hyperbolic systems.

Comparing H -measures and Young measures one sees that the former predicts limits that involve pseudo-differential operators while the latter only yields limits of local expressions (cf. (5.1)). On the other hand the use of H -measures is restricted to quadratic expressions while Young measures can handle arbitrary nonlinearities. A synthesis of the two concepts is a major challenge for the future. So far even a good theory for a trilinear analogue of the H -measure is outstanding. Also the relation between H -measures and Young measures is not known (partial results were obtained by Murat and Tartar [MT 97], [Ta 95]).

As regards length scales, Gérard [Ge 90] introduced a variant of the H -measure, called semiclassical measure, that allows one to study oscillations with a typical length scale $h_j \rightarrow 0$. A similar measure was later considered

by Lions and Paul [LP 93].

A different approach to the resolution of length scales is the notion of two-scale Young measures or Young measures on patterns ([AM 97]). For illustration consider a sequence of periodic functions $w_j : (0, 1) \rightarrow \mathbf{R}$ that is uniformly bounded, $|w_j| \leq M$. For a given sequence of scales $h_j \rightarrow 0$ one defines a new sequence

$$v_j(x, y) = w_j(x + h_j y).$$

For $L > 0$ the set $K = \{g \in L^\infty(-L, L) : |g| \leq M\}$ is a compact subset of $L^\infty(-L, L)$ equipped with the weak* topology and v_j can be viewed as a map

$$\begin{aligned} V_j : (0, 1) &\rightarrow K \\ x &\mapsto v_j(x, \cdot). \end{aligned}$$

Since K is a compact metric space (a subsequence of) the sequence V_j generates a Young measure $\nu : (0, 1) \rightarrow M(K)$. This Young measure (called the two-scale Young measure of the original sequence w_j) is a probability measure on functions, obtained by blowing up the scale h_j . Using this idea one can describe the asymptotic behaviour as $\epsilon \rightarrow 0$ of minimizers of

$$\tilde{I}^\epsilon(u) = \int_0^1 \epsilon^2 u_{xx}^2 + W(u_x) + a(x)u^2,$$

where $0 < c \leq a(x) \leq C$ (cf. section 7.1). If u_{ϵ_j} is a sequence of minimizers, $\epsilon_j \rightarrow 0$, $w_j(x) = \epsilon_j^{-1/3} u_{\epsilon_j}(x)$, $h_j = \epsilon_j^{1/3}$ and ν is the Young measure generated by V_j then $\nu(x)$ is supported on (translates of) sawtooth functions with period $4(2a(x))^{1/3}$ (cf. Theorem 7.1). Two-scale Young measures generalize the concept of two-scale convergence ([Ng 89], [Al 92]) which is very useful if the sequences involved are well approximated by functions that are periodic (with fixed period) in the fast variable.

8.2 Dynamics

So far we have only considered time independent situations and studied minimizers or almost minimizers of the energy. A typical justification is that the time dependent problem admits a natural Liapunov function (free energy, entropy, ...) and therefore the evolution of 'generic' initial data should converge to (at least local) minimizers of the Liapunov functional.

Is such reasoning still reasonable if minimizers of the Liapunov functional do not exist and minimizing sequences have to develop microstructure? Friesecke [Fr 93] and Friesecke and McLeod [FM 96] studied a one dimensional model problem (viscoelastic bar on a foundation) whose Liapunov functional is essentially given by (7.1) (strong convergence of the kinetic energy is easy). They solved a long standing conjecture by showing that the dynamics excludes formation of finer and finer microstructure and hence energy minimization. See Ball et al. [BHJPS 91] and Pego [Pe 87] for related models and Ball [Ba 90] for a general discussion of energy minimization versus dynamics. Virtually nothing is known for the long-time dynamics of higher dimensional models, despite the interesting numerical simulations of Swart [Sw 91].

Another important issue is the evolution of microstructures. If the microstructure at each point in time is described by a Young measure (or some of the objects discussed in section 8.1) is it possible to deduce an evolution law for the Young measure? Conceptually this is similar to the closure problem in turbulence models and one might thus be pessimistic. Nonetheless there has been interesting progress over the last years (see [KP 91], [FBS 94], [HR 94], [De 96], and in particular recent work of Otto [Ot 95], [Ot 97]). An interesting new approach to dynamics that takes into account the presence of many shallow local minima appears in [ACJ 96].

8.3 Computation

Computation of microstructures through numerical energy minimization is a very challenging task. There are presumably many local minimizers for the discrete and the continuous problem, the Euler-Lagrange equations are mixed elliptic-hyperbolic and oscillations typically develop on the scale of the discretization, which renders results very discretization dependent. For a recent review of the state of the art see Luskin [Lu 96] and the references therein. So far, most numerical methods make no use of available analytical information such as the classification of gradient Young measures, the minors relations or algorithms for rank-1 convexification (see sections 1 and 7 of [Lu 96] for the discussion of some exceptions). It seems to me that an important question is how to represent microstructures numerically in an efficient way. Ideally a good representation should both yield a high compression rate and be adapted to the numerical algorithm. This issue is closely related to

the search for better analytical descriptions of microstructure (see section 8.1 above).

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