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Calculus of Variations

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Introduction by the Organisers

The workshop continued the longstanding biannual series at Oberwolfach on Calculus of Variations. This Oberwolfach series provides an important service to the mathematics community, being currently the only periodic international meeting in this very active area.

The main themes of the workshop were variational methods in differential geometry and in nonlinear partial differential equations theory, where exciting topics included geometric flows, condensation and singularity formation in geometric problems, and mass transportation phenomena in partial differential equations.

Among the many traditional and non-traditional application areas of the calculus of variations, the talks covered aspects of general relativity, discrete systems, phase transitions and microstructure, fluid dynamics, quantum chemistry, and approximation theory for rough function spaces.

Workshop: Calculus of Variations

Table of Contents

Rafe Mazzeo	
<i>Constant mean curvature hypersurfaces condensing along a submanifold</i> ..	1545
Antonin Chambolle	
<i>Approximation of SBD functions</i>	1548
Stefan Müller (joint with Nirmalendu Chauduri)	
<i>A rigidity estimate for two incompatible wells</i>	1551
Andrea Braides	
<i>Discrete membranes with defects</i>	1553
Mathieu Lewin	
<i>Solutions of the Multiconfiguration Equations in Quantum Chemistry</i>	1555
Gerhard Huisken	
<i>Variational problems in general relativity</i>	1558
Amandine Aftalion	
<i>Vortex lattices in Bose-Einstein condensates</i>	1559
Irena Fonseca (joint with Massimiliano Morini, Robert Sekerta, and Valeriy Slastikov)	
<i>Equilibria in foams: a phase field model</i>	1559
Robert McCann (joint with Adam Oberman and Maxim Trokhimtchouk)	
<i>Exact semi-geostrophic flows in an elliptical ocean basin</i>	1562
Karsten Matthies (joint with Gero Friesecke)	
<i>Asymptotic profiles of travelling waves in the Fermi-Pasta-Ulam model</i> ...	1563
Marco Cicalese (joint with Andrea Braides)	
<i>Surface energies in discrete systems</i>	1564
Aldo Pratelli (joint with I. Fragal and M.S. Gelli)	
<i>Existence of a continous transport for the Monge problem in R^2</i>	1565
Michael Struwe	
<i>Flow approach to the Niremberg and prescribed Q-curvature problems</i> ..	1567
Sergio Conti	
<i>On the two-well problem with surface energy</i>	1571
Florian Theil	
<i>Crystallisation in two dimensions</i>	1572

Frank Pacard

Compact constant Mean Curvature Surfaces revisited1573

Ernst Kuwert

On solutions of the relative isoperimetric problem1575

Adriana Garroni (joint with C. Francfort)

Quasistatic evolution of damage.....1576

Robert J. Jerrard

Refined Jacobian estimates1577

Bernd Kirchheim (joint with A.Pratelli)

Finite differential inclusion and elliptic regularity1579

Abstracts

Constant mean curvature hypersurfaces condensing along a submanifold

RAFE MAZZEO

There has been substantial progress in the last two decades in the theory of constant mean curvature hypersurfaces in Riemannian manifolds. Roughly speaking, there are two predominant methods for studying the existence and deformation theory: the first draws on techniques from integrable systems, but is effective only when the ambient manifold symmetric, e.g. Euclidean or constant curvature, and is most effective only in low dimensions; the second, relying on various PDE techniques and analytic gluing methods, is more general and flexible. A recent survey of developments in this latter context is contained in the paper [6].

Closely connected to the basic existence problems are questions about the moduli space of all such surfaces, and as part of this it is natural to study the limiting behaviour of sequences of CMC surfaces. As a guide for what to expect, recall that in the closely related study of area minimizing (or stationary) hypersurfaces one has general results from geometric measure theory which ensure compactness in a weak sense, ensuring the existence of possibly singular limits of such sequences. Perhaps a better guide is the study of sequences of (two dimensional) minimal surfaces in three manifolds. Here one has very good compactness theorems if one makes assumptions on the curvature of the ambient space and imposes uniform area bounds on the sequence; without these assumptions, however, as follows from the important work of Colding and Minicozzi, the sequence always limits on a minimal foliation or minimal lamination.

One expects a somewhat similar story for sequences of CMC surfaces, that under favorable conditions and with various strong geometric assumptions, one can extract smooth or nearly smooth limits, and that in general one gets convergence of a subsequence to more complicated object. As an example of a theorem of the first sort, see [2]. The subject of my talk in this Oberwolfach session was a report on some progress in understanding what can happen for more general sequences. This is contained in two recent papers, [7] with Frank Pacard and [8] with Pacard and Fethi Mahmoudi. We consider sequences of CMC hypersurfaces with mean curvature tending to infinity. The easiest example is a family of concentric spheres in \mathbb{R}^n or somewhat more generally, a family of tubes around a linear subspace, in each case with radius tending to zero. Our goal was to understand when such sequences can exist in more general manifolds. More specifically, suppose that Σ is a compact embedded submanifold of arbitrary codimension in the Riemannian manifold (X, g) . The geodesic tubes of radius ρ around Σ are approximately CMC, and we study whether it is possible to perturb this family into a family of exactly CMC hypersurfaces which ‘collapse’ onto Σ .

The case where Σ is a point was studied in the early '90's by Rugang Ye [9], [10], [11]. He proved the following result

Theorem 0.1 (Ye). *Let $p \in X$ be a nondegenerate critical point for the scalar curvature function R_g on X . Then the family of geodesic spheres S_ρ , which form a local foliation around p , can be perturbed to a local foliation where each leaf is a small perturbation of one of these geodesic spheres. Conversely, if M_j is a sequence of CMC surfaces which are diffeomorphically spheres, then subject to some mild extra conditions, M_j collapses to a point p which is a critical point of the scalar curvature function.*

Ye adapted the proof of this result to show the existence of a CMC foliation near infinity in any asymptotically Euclidean manifold. This foliation was obtained by other methods by Huisken and Yau [1], and is important in general relativity.

We generalize this in the

Theorem 0.2. *Suppose that Σ is a nondegenerate compact minimal surface of dimension $k > 0$ in X^{n+1} . Then there is a sequence of disjoint intervals $I_j = [\rho_j^-, \rho_j^+]$ with $\rho_j^\pm \rightarrow 0$ such that for $\rho \in I_j$ the geodesic tube of radius ρ around Σ , $\mathcal{T}_\rho(\Sigma)$, may be perturbed to a CMC hypersurface with mean curvature proportional to $1/\rho$. Moreover, the union of the intervals I_j has density 1 near 0.*

There are two significant differences between the statement of this theorem and Ye's. First, we need no hypotheses concerning the curvature of the ambient manifold at or near Σ ; the minimality of Σ is essentially the replacement for this. Secondly, we can only perturb 'most' geodesic tubes, but do not seem to be able to find CMC tubes at every radius. The fact that there are gaps reflects a genuine bifurcation phenomenon.

The overall idea of the proof is to solve the CMC equation amongst a family of perturbations of these geodesic tubes. These perturbations are obtained by first translating Σ slightly in the normal direction and then taking a normal graph over the resulting surface; thus these perturbations are parametrized by a section Φ of the normal bundle $N\Sigma$, and a function w on $\mathcal{T}_\rho(\Sigma)$. The first main step is to compute the precise asymptotics of the metric and second fundamental form on these perturbed surfaces as a function of ρ , Φ and w . Then one must analyze the linearized mean curvature operator and study its mapping properties in the singular limit as $\rho \rightarrow 0$. There is an infinite sequence of radii $\rho_j \rightarrow 0$ where this linearization becomes degenerate, and the aforementioned gaps are caused by the existence of these degenerate radii. However, avoiding small neighbourhoods of the ρ_j , we are able to carry through the analysis so as to find CMC hypersurfaces in this family of perturbations.

As noted above, the existence of 'degenerate radii' ρ_i is related to a bifurcation phenomenon. This can be seen clearly in the case where Σ is a geodesic circle and X a flat torus. Then the tubes \mathcal{T}_ρ are already CMC, but one also has for each (small) radius ρ other CMC hypersurfaces, namely rescalings of Delaunay surfaces; these are periodic surfaces of revolution and the period of the rescaled surface must match the length of the geodesic. These new families intersect the basic cylindrical family $\mathcal{T}_\rho(\Sigma)$ precisely at the radii ρ_i . In current work of Mahmoudi it is shown

that such Delaunay-type surfaces exist whenever Σ is a nondegenerate geodesic in any manifold X .

Similar bifurcations have been observed in a different context in the work of Malchiodi and Montenegro, cf. [3], [4], [5].

Let S_ρ denote the cylindrical CMC hypersurface obtained by perturbing the geodesic tubes $\mathcal{T}_\rho(\Sigma)$. It follows from our construction that suitable rescalings of the area and curvature densities on S_ρ limit to constant multiples of the standard density on Σ , i.e.

$$\rho^{k-m} \mathcal{H}^m \llcorner S_\rho \rightharpoonup a_1 \mathcal{H}^k \llcorner \Sigma,$$

and, for all $q \geq 1$,

$$\rho^{k-m+q} |A_\rho|^q \mathcal{H}^m \llcorner S_\rho \rightharpoonup a_2 \mathcal{H}^k \llcorner \Sigma,$$

as $\rho \searrow 0$. Here $|A_\rho|^2$ is the norm squared of the second fundamental form on S_ρ , $k = \dim \Sigma$, $m = \dim S_\rho$ and a_1 and a_2 are dimensional constants (a_2 also depends on q).

These equations do not hold for arbitrary families of CMC hypersurfaces condensing on Σ , as illustrated by sequences of collapsing rescaled Delaunay surfaces. In another direction, one should (though this has not been done yet) be able to construct families of CMC hypersurfaces which condense along lower dimensional sets which are still minimal in an appropriate sense, but with singularities, for example a Steiner tree with geodesic edges. A simple example of this is when S_ρ is obtained by homothetically rescaling a fixed Delaunay trinoid in \mathbb{R}^3 . The limit then is a union of three rays meeting at a common vertex, each ray having an associated density coming from the limiting Delaunay necksize on that end; each ray is minimal, of course, and the entire configuration is ‘balanced’ in the sense that the weighted sum of the vectors along the rays vanishes.

Keeping these various phenomena in mind, we make the

Conjecture: *Let S_j be a family of constant mean curvature hypersurfaces with mean curvature $H_j \nearrow \infty$; then for j sufficiently large, S_j is homologically trivial.*

Thus if the S_j were indeed condensing on a lower dimensional (possibly singular) manifold Σ , then S_j should bound a tubular neighbourhood around this condensation set.

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Approximation of *SBD* functions

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Special Bounded Deformation displacements have been introduced by Ambrosio, Bellettini, Dal Maso, Coscia [3, 7] to represent displacements in linearized elasticity problems with discontinuities (that may model cracks in the material). Given $u \in \Omega$, where Ω is an open subset of \mathbb{R}^N , one says that a displacement $u : \Omega \rightarrow \mathbb{R}^N$ has bounded deformation whenever the symmetric part of the distributional derivative $\mathcal{E}(u) = (Du + Du^T)/2$ is a bounded Radon measure. In this case, it is proven in [3] that the measure $\mathcal{E}(u)$ can be decomposed into three parts, one absolutely continuous with respect to the Lebesgue measure dx , denoted by $e(u) dx$, and two other that are singular: a jump part, carried by the rectifiable $(N - 1)$ -dimensional set J_u of points where the function u has two different approximate limits u_+ and u_- , together with a normal vector ν_u , and a “Cantor part”, which vanishes on Borel sets of finite \mathcal{H}^{N-1} measure.

The space $SBD(\Omega)$ is defined as the space of the bounded deformation functions u such that the Cantor part of $\mathcal{E}(u)$ vanishes, so that this measure can be written

$$\mathcal{E}(u) = e(u)(x) dx + (u_+(x) - u_-(x)) \odot \nu_u(x) \mathcal{H}^{N-1} \llcorner J_u(x)$$

where $\mathcal{H}^{N-1} \llcorner J_u$ is the $(N - 1)$ -dimensional Hausdorff measure restricted to J_u and $a \odot b$ denotes the symmetrized tensor product $(a \otimes b + b \otimes a)/2$. It is to *BD* displacements the analogous of the space *SBV* functions to *BV* functions. The space *SBV* has been introduced by Ambrosio and De Giorgi in order to study “free discontinuity” problems arising in image processing [4].

These *SBD* displacements are useful in the theory of brittle crack evolution, following a model proposed by Francfort and Marigo [18, 19]. One can define a “Mumford-Shah”-like potential energy of the form $E(u) = \int_{\Omega} W(e(u)) dx + \mathcal{H}^{N-1}(J_u)$, with W some linearized elasticity bulk energy, and roughly define a discrete evolution with timestep $\delta t > 0$ by letting, for every $n \in \mathbb{N}$, u_n be a minimizer of $E(u)$ among all u with $u = g(n\delta t)$ and $J_{u_n} \supset J_{u_{n-1}}$, where $g(t)$ is a given boundary displacement and the second condition expresses the fact that the

fracture, represented by the jump J_u , is irreversible and can only grow. At this point, several problems arise. Does each minimization problem have a solution? Does there exist some limit evolution as $\delta t \downarrow 0$? Some of these issues are addressed in [2, 15, 11, 17, 13], for variants of this problem (scalar versions, topological restrictions on the cracks, nonlinear elasticity). However, in the case of linearized elasticity, a study of this problem is still out of reach for many technical reasons.

Interesting also would be to find a way to numerically minimize energy E , in order to simulate crack growth. In [8], such experiments have been conducted, that are based on a Ambrosio and Tortorelli [5, 6] approximation of energy E , in the case where W is a positive definite quadratic form of the deformation $e(u)$. But the Γ -convergence of this approximation to E is not known. A major issue is in the proof of the Γ -limsup: in Ambrosio and Tortorelli's works, it relies strongly on the fact that any function in $SBV(\Omega)$ with finite Mumford-Shah energy $\int |\nabla u|^2 + \mathcal{H}^{N-1}(S_u)$ can be approximated by functions u_n such that the jump set S_{u_n} is closed. No such result exists up to now for SBD functions.

In our talk, we have exposed the results of a recent paper [12] (an extension to the N -dimensional case is in preparation) in which we prove such a property. We show that, for W with quadratic growth, provided Ω is bounded and $\partial\Omega$ is locally a subgraph, any $u \in SBD(\Omega) \cap L^2(\mathbb{R}^N)$ with $E(u) < +\infty$ can be approximated (in L^2) by a sequence u_n such that $\limsup_{n \rightarrow \infty} \int_{\Omega} W(e(u_n)) dx + \mathcal{H}^{N-1}(\bar{J}_{u_n}) \leq \int_{\Omega} W(e(u)) dx + \mathcal{H}^{N-1}(J_u)$. It turns out that the jump set J_{u_n} that we build is included in a finite union of closed connected C^1 hypersurfaces, whose total $(N-1)$ -dimensional Hausdorff measure goes to $\mathcal{H}^{N-1}(J_u)$ as $n \rightarrow \infty$.

Using a SBD semicontinuity result proven in [7], our results yields the convergence of $e(u_n)$ to $e(u)$ in L^2 -strong, and the convergence of $\mathcal{H}^{N-1}(\bar{J}_{u_n})$ to $\mathcal{H}^{N-1}(J_u)$. On the other hand, we do not know whether the sequence $(u_n)_{n \geq 1}$ we build can be uniformly bounded in BD . As a consequence we deduce the Γ -convergence of an Ambrosio and Tortorelli [5, 6] approximation of the elasticity Mumford Shah functional, with an L^∞ constraint. This justifies in part the numerical computations presented in [8].

In the talk, we have exposed mainly the simpler " SBV " (scalar) case, for which the result is already well-known. However, all previous proofs in that case relied on a deep theorem of De Giorgi, Carriero and Leaci [16] (see also [14]) on the regularity of minimizers of the Mumford-Shah functional. Our proof is constructive, and can be adapted without great technical difficulties to the SBD case (or other situations with geometrical constraints as in a forthcoming paper with Margherita Solci the from University of Alghero (Sassari, Italy)). It relies first on a discretization argument which is inspired from a work by Gobbi [20] and relies on slicing. A first approximation result is found, but with an approximating sequence (u_n) which is defined on a discrete set of the form $\varepsilon\mathbb{Z} \cap \Omega$. Similar approaches have been used in [10, 1].

Then, the approximate discrete sequence is re-interpolated in Ω using classical linear interpolation, and taking into account the jumps, into a sequence of piecewise continuous functions. This follows an approach introduced in [9] in a similar setting.

A classical difficulty is that in the interpolation process the discontinuity is necessarily approximated in an anisotropic way, hence its measure cannot be correctly reconstructed. This is bypassed by first covering the jump set with finitely many pieces of smooth hypersurfaces, up to a small error of total surface ε , and then performing the above described approximation process. The error in the reconstruction is this time of order $C \times \varepsilon$, and a diagonalization argument yields the final result—with an error that goes to zero.

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A rigidity estimate for two incompatible wells

STEFAN MÜLLER

(joint work with Nirmalendu Chauduri)

A classical result in geometry and continuum mechanics states that if a Lipschitz maps satisfies $\nabla u \in SO(n)$ almost everywhere then the gradient is in fact (locally) constant. The following quantitative version has been established recently and has lead to a rigorous derivation of a hierarchy of plate theories from three-dimensional nonlinear elasticity.

Theorem 1 ([8]) *Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain, $n \geq 2$. There exists a constant $C(\Omega)$ with the property that for each $u \in W^{1,2}(\Omega, \mathbb{R}^n)$, there exists an associated rotation $R \in SO(n)$, such that*

$$(0.1) \quad \|\nabla u - R\|_{L^2(\Omega)} \leq C(\Omega) \|\text{dist}(\nabla u, SO(n))\|_{L^2(\Omega)}.$$

This generalizes a classical result of F. John [9] who derived an estimate of $\|\nabla u - R\|_{L^2}$ in terms of $\|\text{dist}(\nabla u, SO(n))\|_{L^\infty}$ for locally Bilipschitz maps u .

In connection with mathematical models for materials undergoing solid-solid phase transformations [1, 4, 7] one is interested in deformations u whose gradient is close to a set $K := \cup_{i=1}^m SO(n)U_i$, which consists of several copies of $SO(n)$ (so-called energy wells). Here we consider the two-well problem for two *strongly incompatible* wells. For further information on the two-well problem see [6, 10, 12]. Rigidity for a linearized version of the two-well problem is discussed in [5]. We prove an estimate of the type (0.1) for two strongly incompatible wells.

Theorem 2 ([3]) *Let $\Omega \subset \mathbb{R}^n$ be a bounded Lipschitz domain, $n \geq 2$ and $K := SO(n) \cup SO(n)H$, where $H = \text{diag}(\lambda_1, \dots, \lambda_n)$, $\lambda_i > 0$ such that $\sum_{i=1}^n (1 - \lambda_i)(1 - \det H/\lambda_i) > 0$. There exists a positive constant $C(\Omega, H)$ with the following property. For each $u \in W^{1,2}(\Omega, \mathbb{R}^n)$ there is an associated $R := R(u, \Omega) \in K$ such that*

$$(0.2) \quad \|\nabla u - R\|_{L^2(\Omega)} \leq C(\Omega, H) \|\text{dist}(\nabla u, K)\|_{L^2(\Omega)}.$$

Theorem 2 has interesting consequences for the scaling of the energy in thin martensitic films [2, 11]. There are examples such that the two-wells are strongly incompatible in three dimensions (in the sense above) but compatible in two dimensions. Using Theorem 2 one can show that in this case the optimal energy

per unit film thickness of the order of the film thickness h (provided that the two-dimensional limit uses both wells). This is a nonstandard scaling which lies in between the usual membrane theory (scaling of order 1) and the bending (Kirchhoff-Love) theory (scaling of order h^2).

The above condition on H is related to the following result of Matos.

Lemma 3 ([10]) *Let $K := SO(n) \cup SO(n)H$, $H = \text{diag}(\lambda_1, \dots, \lambda_n)$, $\lambda_i > 0$. Then there exists a smooth function $W : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$, which is uniformly convex and has quadratic growth and satisfies $\nabla W = \nabla \det = \text{cof}$ in K , if and only if $\sum_{i=1}^n (1 - \lambda_i)(1 - \det H/\lambda_i) > 0$.*

Using Matos' result and elliptic regularity theory one sees easily that every map whose gradient lies exactly in K must be in $W^{2,2}$. Hence the gradient must lie in one of the connected components $SO(3)$ or $SO(3)H$ and is therefore constant by the classical rigidity result.

To prove Theorem 2 one needs a quantitative version of this. To this end one uses a result of Luckhaus, which states that a function which is close to characteristic function in L^1 and which has controlled $W^{1,2}$ norm must be close to 0 or 1. Finally one uses a covering argument to improve the exponent in the Luckhaus estimate to the optimal scaling in Theorem 2.

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Discrete membranes with defects

ANDREA BRAIDES

We are interested in describing the overall properties of a membrane in which a distribution of ‘defects’ is taken into account. We find it convenient to introduce a discrete model, whose properties are then described by a suitable continuous counterpart.

The free energy of a two-dimensional discrete membrane with a bounded open set $\Omega \subset \mathbb{R}^2$ as reference configuration is modelled by a functional

$$(0.1) \quad E_\varepsilon(u) = \frac{1}{2} \sum_{|i-j|=\varepsilon} \phi_{ij}^\varepsilon(u_i - u_j),$$

where $u : \varepsilon\mathbb{Z}^2 \cap \Omega \rightarrow \mathbb{R}$ represents the vertical displacement of the membrane and $u_i = u(i)$. If we think of this as a mass-spring system then ϕ_{ij}^ε represents the energy density of the interactions between the two point masses parameterised by i and j in the reference configuration (note that we only take into account *nearest neighbours*). The small positive parameter ε is introduced so that averaged properties of E_ε are described by its Γ -limit F (see e.g. [3, 10]). Note that this problem can be framed within the recent applications of Γ -convergence to the description of the passage from discrete systems to continuous variational problems (see e.g [5, 7])

We suppose that the functions ϕ_{ij}^ε may take two forms:

(1) (*strong springs*) $\phi_{ij}^\varepsilon(z) = z^2$. If only strong springs are present E_ε is nothing but a finite-difference approximation of the *Dirichlet integral*, and $F(u) = \int_\Omega |\nabla u|^2 dx$ is defined on $H^1(\Omega)$;

(1) (*weak springs*) $\phi_{ij}^\varepsilon(z) = \min\{z^2, \varepsilon\}$. In terms of the difference quotient we may write

$$(0.2) \quad \phi_{ij}^\varepsilon(u_i - u_j) = \varepsilon f\left(\varepsilon \left(\frac{u_i - u_j}{\varepsilon}\right)^2\right) = \begin{cases} (u_i - u_j)^2, & \text{if } \frac{u_i - u_j}{\varepsilon} \leq \frac{1}{\sqrt{\varepsilon}} \\ 1, & \text{otherwise,} \end{cases}$$

where $f(w) = \min\{|w|, 1\}$. We may interpret the energy ϕ_{ij}^ε as describing an elastic spring until the gradient reaches the threshold $1/\sqrt{\varepsilon}$, after which the spring is broken. Note that this value gives the only interesting scaling for the fracture threshold. If only weak springs are present then the Γ -limit is finite on the space $SBV(\Omega)$ (see [2]) and is the *weak membrane energy*

$$(0.3) \quad F(u) = \int_\Omega |\nabla u|^2 dx + \int_{S(u)} \|\nu\|_1 d\mathcal{H}^1,$$

where $\|\nu\|_1 = |\nu_1| + |\nu_2|$ (see Chambolle [9]). F may be interpreted as an anisotropic Griffith fracture energy (see [11]), the anisotropy clearly deriving from the square lattice symmetries.

We consider the case when

$$(0.4) \quad \phi_{ij}^\varepsilon(z) = \begin{cases} \varepsilon f(\varepsilon z^2), & \text{with probability } p \\ z^2 & \text{with probability } 1 - p. \end{cases}$$

This can be done by introducing suitable i.i.d. random variables (see [8]) corresponding to a *bond-percolation model* (see e.g. [12]). With fixed a realisation ω we will write E_ε^ω to highlight the fixed choice of ϕ_{ij}^ε in terms of ω , and F^ω the corresponding Γ -limit. The following theorem holds [8].

Theorem (Braides and Piatnitsky).

(i) **(subcritical regime)** *If $p < 1/2$ then almost surely the limit is finite only on $H^1(\Omega)$ and*

$$(0.5) \quad F^\omega(u) = \int_{\Omega} |\nabla u|^2 dx$$

independently of ω ;

(ii) **(supercritical regime)** *If $p > 1/2$ then there exists $g_p \leq c < +\infty$ such that almost surely*

$$(0.6) \quad F^\omega(u) \leq \int_{\Omega} |\nabla u|^2 dx + \int_{S(u)} g_p(\nu) d\mathcal{H}^1.$$

Remark. (i) the threshold $1/2$ corresponds to the *bond-percolation threshold* in dimension 2. Other choices of percolation models (e.g. site percolation) are possible; the results are exactly the same but with the corresponding percolation threshold in place of $1/2$;

(ii) even if no assumptions on the distribution of weak and strong springs are made, by using the localisation methods of Γ -convergence (see e.g. [3] Chapter 16) applied to the passage from discrete to continuous energies (as in [1] in the case of Sobolev-type growth conditions; see also [4]) it is possible to show that F always has an integral representation on $SBV(\Omega)$. By comparison with the Dirichlet integral and with the weak membrane energy the bulk energy density is bound to be $|\nabla u|^2$, and we have that

$$(0.7) \quad F^\omega(u) = \int_{\Omega} |\nabla u|^2 dx + \int_{S(u)} g(x, u^+ - u^-, \nu) d\mathcal{H}^1;$$

(iii) note that it is not possible to obtain meaningful *bounds* on g in terms of the local limit density of weak/strong connections as those obtained in [6] when considering mixtures of strong springs with two possible choices of elastic moduli. In fact, it can be shown that the only bound we may obtain is the trivial one: $g(x, w, \nu) \geq \|\nu\|_1$. If we are in a *homogenization* setting, i.e. a periodicity assumption is made, then *homogenization formulas* for g can be proved.

Remark. The proof uses the Γ -convergence techniques for free-discontinuity problems combined with percolation theory. In particular in the subcritical regime one uses the properties of the ‘strong cluster’ to obtain the coerciveness in $H^1(\Omega)$, while in the supercritical regime one constructs recovery sequences using connections on the ‘weak cluster’ to approximate discontinuity sets. It seems likely that this is almost surely the optimal way to approximate jump sets. We are then led to the following conjecture.

Conjecture: *The upper bound in (0.6) is optimal; i.e. the Γ -limit is independent of ω and is given by the right-hand side of (0.6), with g_p suitably defined by a least-path problem on the weak cluster (see [8]).*

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Solutions of the Multiconfiguration Equations in Quantum Chemistry

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The multiconfiguration methods are the natural generalization of the well-known Hartree-Fock theory for the description of non-relativistic electrons in atoms and molecules. We present here our latest results regarding the existence of minimizers and of saddle points [9, 5].

Let us consider a molecule which contains

- M nuclei treated as pointwise classical particles of charges Z_1, \dots, Z_M which are clamped at positions $R_1, \dots, R_M \in \mathbb{R}^3$, and with total charge $Z := \sum_{m=1}^M Z_m$. They create the electrostatic potential $V(x) = -\sum_{m=1}^M \frac{Z_m}{|x-R_m|}$.
- N non-relativistic electrons described by a normalized wavefunction

$$\Psi(x_1, \dots, x_N) \in L_a^2((\mathbb{R}^3)^N, \mathbb{R}).$$

The subscript a indicates that, due to the Pauli principle, we solely consider wavefunctions which are antisymmetric under permutations of variables, i.e.

$$\Psi(x_1, \dots, x_N) = \epsilon(\sigma)\Psi(x_{\sigma(1)}, \dots, x_{\sigma(N)})$$

a.e. for all $\sigma \in S_N$.

The energy of the electrons in the quantum state Ψ is $\mathcal{E}(\Psi) = \langle \Psi, H_N \Psi \rangle$ where H_N is the purely Coulombic N -body Hamiltonian

$$H_N = \sum_{i=1}^N \left(-\frac{1}{2} \Delta_{x_i} + V(x_i) \right) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|}.$$

When $Z > N - 1$, the spectrum of H_N has the form $\sigma(H_N) = \{\lambda_d\} \cup [\Sigma; +\infty)$ where the λ_d 's are eigenvalues of finite multiplicity, converging to Σ as $d \rightarrow \infty$, and where $\Sigma < 0$ when $N \geq 2$. A normalized eigenfunction associated with λ_1 is called a ground state. Higher eigenfunctions are called excited states. In practice, this model is out of reach due to the excessive dimension of the space \mathbb{R}^{3N} on which the wavefunctions are defined. Therefore, the multiconfiguration (MC) approximation is often used by chemists. In this case, one restricts the set of admissible wavefunctions Ψ to those which are a finite combination of Slater determinants. They take the form

$$(0.1) \quad \Psi = \sum_{1 \leq i_1 < \dots < i_N \leq K} c_{i_1 \dots i_N} \phi_{i_1} \wedge \dots \wedge \phi_{i_N}$$

where $\phi_1 \wedge \dots \wedge \phi_N(x_1, \dots, x_N) := (N!)^{-1/2} \det(\phi_i(x_j))$. Due to the normalization constraint on Ψ , we introduce the following manifold

$$\mathcal{M}_N^K = \left\{ (c, \Phi) \in \mathbb{R}^{\binom{K}{N}} \times (H^1(\mathbb{R}^3))^K, \sum (c_{i_1 \dots i_N})^2 = 1, \int_{\mathbb{R}^3} \phi_i \phi_j = \delta_{ij} \right\}.$$

The energy is simply defined on M_N^K by $E_N^K(c, \Phi) = \langle \Psi, H_N \Psi \rangle$, where Ψ is given by formula (0.1). We refer the reader to [5] for an explicit expression of E_N^K in terms of c and Φ . E_N^K is non-quadratic and the associated Euler-Lagrange equations form a complicated system of coupled non-linear PDEs.

When $K = N$, we recover the celebrated Hartree-Fock approximation for which it is known that a minimizer exists [7, 8]. In [8], a sequence $(\Phi^n)_{n \in \mathbb{N}}$ of critical points of $E_N^N(1, \cdot)$ has been constructed, but these solutions cannot be interpreted as approximate excited states since they satisfy $E_N^N(1, \Phi^n) \rightarrow_{n \rightarrow \infty} 0$, whereas $\lambda_d \rightarrow \Sigma < 0$ as $d \rightarrow \infty$. The first result on a MC method is due to Le Bris [4] who proved the existence of a minimizer on a subset of M_N^{N+2} . Finally, the existence of a minimizer of E_N^K on M_N^K for any $K \geq N$ has been recently proved by Friesecke [2]. However his geometrical method is not adapted to obtain critical points.

In [9, 5], we propose a new method of proof which can be also used to obtain critical points. It is inspired by [8] (we prove the compactness of Palais-Smale sequences with a Morse information).

Theorem 1 (Existence of minimizers and of infinitely many critical points for each K , [5]). *Assume that $Z > N - 1$ and $K \geq N$. Then,*

- (1) *there exists a minimizer of E_N^K on M_N^K ;*
- (2) *there exists a sequence $(\tilde{c}^n, \tilde{\Phi}^n)$ of critical points of E_N^K on M_N^K such that $\lim_{n \rightarrow +\infty} E_N^K(\tilde{c}^n, \tilde{\Phi}^n) = 0$.*

This result can be extended to more practical methods in which only some well-chosen Slater determinants are selected (see [5] for details).

Like for [8], the $(\tilde{c}^n, \tilde{\Phi}^n)$ cannot be interpreted as excited states. Numerically, it is observed that E_N^K possesses a lot of critical points on M_N^K (due to the non-linearity) and it seems very difficult to identify the ones that can be interpreted as approximate excited states of the molecule. In [5], we have constructed for each K a finite number of critical points that have this property.

Theorem 2 (Existence of approximate excited states, [5]). *Assume that $Z > N - 1$ and $K \geq N$. Then, there exists a sequence $(c_d, \Phi_d) \in M_N^K$ for $d = 1, \dots, \binom{K}{N}$ of critical points of E_N^K on M_N^K , with a Morse index at most $d - 1$, which fulfills, denoting $\lambda_d^K = E_N^K(c_d, \Phi_d)$,*

$$\lambda_d \leq \lambda_d^K \quad \text{and} \quad \lim_{K \rightarrow +\infty} \lambda_d^K = \lambda_d.$$

These points are constructed by inf – sup type methods on homotopic families of dimension d , which are invariant under a certain action of the group \mathbb{Z}_2 , in the spirit of [8, 3]. For $d = 2$ (first excited state), we have

$$\lambda_2^K = \inf_{(c, \Phi) \in M_N^K} \left\{ \inf_{\gamma \in \Gamma_{(c, \Phi)}} \max_{t \in [0; 1]} E_N^K(\gamma(t)) \right\}$$

$$\Gamma_{(c, \Phi)} = \left\{ \gamma \in C^0([0; 1], M_N^K), \gamma(0) = (c, \Phi), \gamma(1) = (-c, \Phi) \right\}.$$

Numerically, the first inf can be simplified by simply taking $(\bar{c}, \bar{\Phi})$, a global minimizer of E_N^K on M_N^K . The procedure in brackets is then simply a mountain-pass method between $(\bar{c}, \bar{\Phi})$ and $(-\bar{c}, \bar{\Phi})$. This method mimics the classical formula which allows to obtain λ_2 in the linear setting as a mountain pass between Ψ_1 and $-\Psi_1$ where $H_N \Psi_1 = \lambda_1 \Psi_1$. This totally new definition gives rise to a novel algorithm for the computation of the first excited state of molecules, described and tested in [1, 6].

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Variational problems in general relativity

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Let (M^3, g, K) be an initial data set, ie (M^3, g) is a complete Riemannian manifold and K is an additional symmetric tensorfield on M^3 . The data g and K are motivated by the induced metric and second fundamental form of a spacelike hypersurface in a Lorentzian 4-manifold modelling an isolated gravitating system such as for example a star, a binary or a black hole. For an isolated system the data are assumed to be asymptotically flat, ie the noncompact part(s) of (M^3, g, K) is (are) assumed to be diffeomorphic to $R^3 - B_1(0)$ with data g, K approaching the standard data of a plane in Minkowski space at a certain rate.

The lecture explains how geometric variational principles can be used to construct special 2-spheres near infinity in (M^3, g, K) if a certain geometric invariant of M^3, g , called the mass of the system is positive. The special 2-spheres typically are surfaces of constant mean curvature H , solutions to inverse mean curvature flow or Willmore surfaces of given area. One part of the lecture explains recent results of Jan Metzger, (Tübingen) [M], on the existence of 2-spheres satisfying $H + tr_{Sigma} = const$ and $H - tr_{Sigma} = const$. assuming much milder decay conditions on g and K than previous work by Huisken and Yau [HY] on cmc-surfaces. The relation of this work to recent quantitative rigidity estimates of Müller and DeLellis [LM] and to results on the behaviour of solutions to the inverse mean curvature flow by Huisken and Ilmanen [HI1],[HI2] is also explained.

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Vortex lattices in Bose-Einstein condensates

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Vortices in Bose Einstein condensates: One of the key issues related to superfluidity is the existence of quantized vortices. We present very recent experiments on Bose-Einstein condensates exhibiting vortices, which consist in rotating the trap holding the atoms. We investigate the behavior of the wave function which minimizes the Gross Pitaevskii energy. This energy takes into account the special shape of the trapping potential. In a regime with a small parameter, we give a simplified expression of the energy which only depends on the number and shape of vortex lines. This allows us to study in detail the structure of the lines which have either a U or S shape and compare with experiments. We also present results where the type of trapping potential can be at the origin of multiply quantized vortices. Finally, we describe the regime of rapid rotation where a dense vortex lattice is observed. The particularity of this lattice is to be distorted towards the edges. Using double scale convergence, we show why the distorted lattice has a lower energy than a regular lattice.

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Equilibria in foams: a phase field model

IRENA FONSECA

(joint work with Massimiliano Morini, Robert Sekerta, and Valeriy Slastikov)

The role of surfactants in stabilizing, and possibly encouraging, the formation of bubbles in foams, is studied using a phase-field model. Ultimately, the goal is to treat solid (metallic) foams, such as AL_2O_3 , with important applications in industry such as the manufacturing of lightweight sandwich structures in automotive industry, and in biotechnology, for example in the making of highly porous scaffolds for bone tissue engineering. Most research has focused on aqueous foams

(shampoo, dishwasher detergent, beer, soap froth, etc.), with some incursions into polymeric foams, but the realm of solid foams has been virtually untouched by a rigorous mathematical treatment. In solid foams anisotropy plays a very important role in determining the polyhedral shapes in cellular packing, and an important analytical and geometrical challenge is to explain the different sizes of clusters in cellular packing (see [3], [18], [16], [20], [19]).

Here we address solid foams, but our initial quest as outlined above is one where an isotropic framework is justifiable. It is commonly agreed that formation of bubbles is intrinsically related to phase transitions phenomena, and that solid foams and liquid foams share many topological and geometrical properties, due in part to the fact that solid foams typically evolve in the fluid state as gas bubbles, expanding and deforming under the influence of viscous forces, surface tension, surfactants, etc. For this reason, the model adopted in this paper is a modification of van der Waals-Cahn-Hilliard's model for fluid-fluid phase transitions (see [1], [5], [6], [7], [8], [9], [12], [13], [14], [15], [21], [22], [23], [24], [25]; for related issues within the realm of the Eikonal equation we refer to [2], [4], [17]), with an added term that accounts for the influence of the surfactant in preventing coalescence of bubbled and in encouraging the formation of interfaces.

With $\Omega \subset \mathbb{R}^N$ a bounded, open set, denoting the ambience space, $u : \Omega \rightarrow \mathbb{R}$ the phase-field that takes values 1 in the gas, 0 in the air then the transition between phases occurs across a thin fluid layer penalized by a (surface) gradient term, and we consider a double-well potential $f : \mathbb{R} \rightarrow [0, +\infty)$ with $\{f = 0\} = \{0, 1\}$ that drives the system to the two phases. The total energy of the system, after rescaling, reads

$$G_\epsilon(u, \rho) := \frac{1}{\epsilon} \int_\Omega f(u) dx + \epsilon \int_\Omega |\nabla u|^2 dx + \alpha(\epsilon) \int_\Omega (\rho - |\nabla u|)^2 dx,$$

where $\rho : \Omega \rightarrow [0, +\infty)$ stands for the surfactant, and $\alpha(\epsilon) \rightarrow 0^+$. The volume of surfactant is given a priori and so is the total volume of gas bubbles. The main analytical objective in this paper is to identify the asymptotic behavior of equilibria. Precisely, if $(u_\epsilon, \rho_\epsilon)$ minimizes G_ϵ then can we establish that $\{(u_\epsilon, \rho_\epsilon)\}$ converges to some macroscopic state (u, ρ) , and, if yes, what characterizes (u, ρ) , e.g. does (u, ρ) minimize a new, macroscopic (relaxed) energy? The analysis shows that the regime of interest, both mathematically as well as when confronted with experimentation, is that where $\alpha(\epsilon)$ is of the same order of ϵ . In this case, with $\alpha(\epsilon) = \epsilon$, it is shown that G_ϵ Γ -converges (with respect to $L^1 \times$ (weak-*) convergence; see [10], [11]) to

$$F(u, \mu) := \begin{cases} \int_{S_u} \phi \left(\frac{d\mu}{d\mathcal{H}^{N-1}|_{S_u}}(x) \right) d\mathcal{H}^{N-1}(x) & \text{if } u \in BV(\Omega; \{0, 1\}), \\ +\infty & \text{otherwise,} \end{cases}$$

where ϕ is a non-increasing, convex, surface energy density such that

$$(0.1) \quad \phi(0) = 2\sqrt{2} \int_0^1 \sqrt{f(s)} ds, \quad \phi(\gamma) = 2 \int_0^1 \sqrt{f(s)} ds \quad \text{for } \gamma \geq 1.$$

We observe that

- the macroscopic energy F is only sensitive to the restriction of μ to the interface S_u , and we interpret this fact by saying that the surfactant segregates to the interface;
- F remains unchanged if the density of the surfactant μ on the interface S_u , $\frac{d\mu}{d\mathcal{H}^{N-1}}$, exceeds 1. Indeed, in view of (0.1) the energy is impervious to adding more surfactant and the system reaches saturation;
- looking at F now as having the location of the surfactant established from the onset, by a direct inspection of F it is now clear that this determines the locus of interface formation;
- the decreasing nature of φ leads us to believe (although this warrants a future rigorous analytical verification) that it may be energetically more favorable to spread a small amount of surfactant over a bigger number of smaller bubbles than to spread an even smaller and thinner amount of surfactant over fewer, bigger bubbles;
- the model adopted indeed explains why the presence of surfactant makes it energetically more favorable to create bubbles. This is of the utmost importance in applications as the usage of foams depends in a crucial way on their wetness.

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Exact semi-geostrophic flows in an elliptical ocean basin

ROBERT MCCANN

(joint work with Adam Oberman and Maxim Trokhimtchouk)

A new family of exact solutions is analyzed, which model 2D circulations of an ideal fluid in a uniformly rotating elliptical tank, under the semi-geostrophic approximation from meteorology and oceanography. The fluid pressure and stream function remain quadratic functions of space at each instant in time, whose fluctuations are described by a single degree of freedom Hamiltonian system depending on two conserved parameters: domain eccentricity and the constant value of potential vorticity. These parameters determine the presence or absence of periodic orbits with arbitrarily long periods, fixed points of the dynamics, and aperiodic homoclinic orbits linking hyperbolic saddle points. The energy relative to these parameters selects the frequency and direction in which isobars nutate or precess, as well as the steady circulation direction of the fluctuating flow. The canonically conjugate variables are the moment of inertia and angle of inclination of an elliptical inverse-potential-vorticity patch evolving in dual coordinates.

Asymptotic profiles of travelling waves in the Fermi-Pasta-Ulam model

KARSTEN MATTHIES

(joint work with Gero Friesecke)

In joint work with Gero Friesecke, we analyse the behaviour of travelling waves in the Fermi-Pasta-Ulam system described by the energy

$$(0.1) \quad H = \sum_{n \in \mathbb{Z}} \left(\frac{1}{2} p_n^2 + V(q_{n+1} - q_n) \right)$$

which gives the dynamics as

$$(0.2) \quad \dot{q}_n = p_n, \quad \ddot{q}_n = \dot{p}_n = V'(q_{n+1} - q_n) - V'(q_n - q_{n-1}).$$

This describes a one-dimensional monatomic chain (with p_n, q_n denoting the momentum and displacement of the n^{th} atom)

A key physical requirement of the interaction potential V is that it is minimized when neighbouring particles are placed at some equilibrium distance $d > 0$, and that it tends to infinity as the neighbour distance tends to zero. Since the particle positions x_n corresponding to displacements q_n are $x_n = nd + q_n$ ($n \in \mathbb{Z}$), this means that $V(r)$ must have a minimum at $r = 0$ and that $V(r) \rightarrow \infty$ as $r \rightarrow -d$. More precisely we assume:

- (H1) (Minimum at zero) $V \in C^3(-d, \infty)$, $V \geq 0$, $V(0) = 0$, $V''(0) > 0$
- (H2) (Growth) $V(r) \geq c_0(r + d)^{-1}$ for some $c_0 > 0$ and all r close to $-d$ and $V(r) = \infty$ for $r \leq -d$.
- (H3) (Hardening) $V'''(r) < 0$ in $(-d, 0]$, $V(r) < V(-r)$ in $(0, d)$.

We are interested in travelling waves $q_n(t) = q(n - ct)$, the equations of motion reduce to the scalar second-order differential-difference equation

$$(0.3) \quad c^2 q''(x) = V'(q(x + 1) - q(x)) - V'(q(x) - q(x - 1)).$$

such waves have been rigorously proven to exist for generic nonlinear potentials V . The construction in [FW94] is based on the variational principle

$$(0.4) \quad \begin{aligned} &\text{Minimize } T(q) := \frac{1}{2} \int_{\mathbb{R}} q'(x)^2 dx \text{ among } q \in W_{loc}^{1,2}(\mathbb{R}) \text{ satisfying} \\ &q' \in L^2(\mathbb{R}), U(q) := \int_{\mathbb{R}} V(q(x + 1) - q(x)) dx = K. \end{aligned}$$

The goal is to determine the Γ -limit of the variational problem and the limiting profile in the high-energy regime, for Lennard-Jones type interactions. Since this regime is highly discrete and involves strong forces, neither classical continuum approximations nor weak coupling approximations are possible.

Prototypical are the standard Lennard-Jones potentials

$$V(r) = a \left((r + d)^{-m} - d^{-m} \right)^2 \text{ for } r > -d, \quad a > 0, \quad m \in \mathbb{N}.$$

The limiting profile for $K \rightarrow \infty$ was derived in [FM02]. Here we recover this as a corollary of the following Γ -convergence result. We let

$$W_0 := \{q \in W_{loc}^{1,2}(\mathbb{R}) \mid q(0) = 0, q' \in L^2(\mathbb{R})\},$$

for every displacement profile q , we denote the relative displacement profile as $r(\cdot) = q(\cdot + 1) - q(\cdot)$. As in (0.4) we will consider the functional T on

$$\begin{aligned} X_K &= \{q \in W_0 \mid U(q) = K\} \\ X_\infty &= \{q \in W_0 \mid r(x) \geq -d \forall x \in \mathbb{R}; \\ &\quad \exists \text{ compact nonempty set } S_q \subset \mathbb{R} \text{ with } r|_{S_q} = -d\} \end{aligned}$$

Theorem 1. (Γ -convergence) *Assume that the interaction potential satisfies (H1), (H2). Then the problem*

$$(0.5) \quad \text{Minimize } T(q) \text{ for } q \in X_K$$

Γ -converges to the problem

$$(0.6) \quad \text{Minimize } T(q) \text{ for } q \in X_\infty,$$

in the following sense

- (1) (lim-inf-inequality) *If $q^{(K)} \rightharpoonup q$ in W_0 with $q^{(K)} \in X_K$, $q^{(K)}$ translation normalized (i.e. $r^{(K)}(0) = \min_{x \in \mathbb{R}} r^{(K)}(x)$), then $q \in X_\infty$ and $T(q) \leq \liminf_{K \rightarrow \infty} T(q^{(K)})$,*
- (2) (Existence of recovery sequence) *For all $q \in X_\infty$ there exists a sequence $q^{(K)} \in X_K$ with $q^{(K)} \rightharpoonup q$ in W_0 and $T(q^{(K)}) \rightarrow T(q)$.*

A consequence is the asymptotic profile

Corollary 1. (*Asymptotic shape of minimizers*) *Every translation normalized sequence $q^{(K)}$ of minimizers of T on X_K converges in W_0 weakly to the up to translation unique minimizer of the limit problem*

$$q_\infty(x) := \begin{cases} 0, & x \leq 0 \\ -dx, & x \in [0, 1] \\ -d, & x \geq 1. \end{cases}$$

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Surface energies in discrete systems

MARCO CICALESE

(joint work with Andrea Braides)

Non-convex interactions in lattice systems lead to a number of interesting phenomena that can be translated into a variety of energies within their limit continuum

description as the lattice size tends to zero. These effects may be due to different superposed causes.

The simplest case is when only nearest-neighbour interactions are present, in which case the bulk energy density of the limit problem is computed via a convexification formula ([1]). When not only nearest-neighbour interactions are taken into account, in contrast, the description of the limit problem turns out more complex involving in general some ‘homogenization’ process ([4], [1]).

In a joint work with Andrea Braides, we provide a higher-order description of next-to-nearest-neighbour systems, using the terminology of developments by Γ -convergence (introduced in Azellotti Baldo [2]) and equivalence of variational theories (developed by Braides Truskinovsky [5]). We deal with the one-dimensional case in which the limit bulk energy density is described by a formula of ‘convolution type’ that highlights a non-trivial balance between first and second neighbours ([6], [3]) and an easier description of the phenomena is possible. Besides the possibility of oscillatory solutions on the microscopic scale, we show some additional features: first, the appearance of a boundary-layer contribution on the boundary due to the asymmetry of the boundary interactions; second, the appearance of a phase-transition surface energy, that is due to the non convexity of the bulk energy density that force the production of phase transitions and the appearance of internal boundary layers due to the presence of next-to-nearest neighbour interactions. By showing an equivalent family of continuum energies we highlight that second neighbours play the same role as the higher-order gradients in the gradient theory of phase transitions.

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Existence of a continuous transport for the Monge problem in R^2

ALDO PRATELLI

(joint work with I. Fragal and M.S. Gelli)

The transport problem, first proposed by G. Monge in 1781, consists in minimizing the *cost* of some *transports*. The data are two given probability measures

f^+ and f^- on \mathbb{R}^2 , and the transports are the Borel maps $t : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ such that $t_{\#}f^+ = f^-$. To each transport one associates the cost

$$\mathbb{C}(t) := \int_{\mathbb{R}^2} |t(x) - x| df^+(x),$$

and the goal of the transport problem is to find a transport t minimizing the cost \mathbb{C} . Much more general versions of the problem are often considered, replacing \mathbb{R}^2 by \mathbb{R}^N or some general metric space X , and the Euclidean norm $|\cdot|$ by the square $|\cdot|^2$ or some general l.s.c. function $c(x, t(x))$. Even though the setting of the problem is so simple, it has not been easy to understand hypotheses under which the existence of an optimal transport is ensured –in general, there may easily be no optimal transports or even no transports at all. The first existence result (valid in any \mathbb{R}^N with the Euclidean norm) has been found by Evans and Gangbo [3], and later sharpened by Caffarelli, Feldmann and McCann [2], by Trudinger and Wang [5] and by Ambrosio [1]. The more general version we have now states the existence of an optimal transport if f^+ is absolutely continuous with respect to the Lebesgue measure and if the first order moments of f^{\pm} are finite.

Since nothing were known about the regularity of the optimal transports, we decided to investigate how regularity assumptions on f^{\pm} can provide regularity to some optimal transport. We proved [4] a continuity assert for a particular optimal transport (it is easy to see that there are many different optimal transports and that many of them are no more regular than Borel maps):

Theorem 0.3. *Assume that f^{\pm} are absolutely continuous with respect to the Lebesgue measure, that f^{\pm} are two compact, convex and disjoint subsets of \mathbb{R}^2 , and that the densities of f^{\pm} are continuous functions on f^{\pm} and strictly positive on $(f^{\pm})^0$. Then there exists a continuous optimal transport.*

To show our result, we reduced to check a couple of geometrical properties, and this reduction is true in any \mathbb{R}^N ; however, the hard part of the construction is to show that these two properties are true, and we only proved this fact in \mathbb{R}^2 . Our work contains also a number of examples to understand the behaviour of the optimal transports we have in mind, and to realize that the hypotheses, which could seem too strong at first glance, are in fact quite reasonable and fairly optimal.

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Flow approach to the Nirenberg and prescribed Q-curvature problems

MICHAEL STRUWE

1. INTRODUCTION

A famous problem posed by Louis Nirenberg is the question which functions $f: S^2 \rightarrow \mathbb{R}$ arise as the Gaussian curvature of a conformal metric g on S^2 . Necessary conditions follow from the Gauss-Bonnet theorem

$$(1.1) \quad \int_{S^2} K \, d\mu_g = 4\pi$$

and the Kazdan-Warner [13] identity

$$(1.2) \quad \int_{S^2} \langle \nabla K, \nabla x_i \rangle_{g_{S^2}} \, d\mu_g = 0, \quad 1 \leq i \leq 3,$$

where g_{S^2} is the standard spherical metric on $S^2 = \{x = (x_1, x_2, x_3) \in \mathbb{R}^3; |x| = 1\}$ and where K is the Gauss curvature of g . Here we identify the restrictions of the coordinate functions x_i with the eigenfunctions $\varphi_i(x) = x_i$ of the Laplace operator on (S^2, g_{S^2}) , satisfying $\Delta_{g_{S^2}} \varphi_i + 2\varphi_i = 0$, $i = 1, 2, 3$. In particular, no function $f \leq 0$ and no function $f = \psi \circ x_i$, where ψ is a monotone function on $[-1, 1]$, can be realized as the Gauss curvature of a conformal metric g on S^2 .

On the other hand, numerous sufficient conditions are known, beginning with the following result of Chang-Yang [7].

Theorem 1.1. *Let f be a positive, smooth function with only non-degenerate critical points. Suppose there are at least two local maxima of f , and at all saddle points Q of f there holds $\Delta f(Q) > 0$. Then f is the Gauss curvature of a conformal metric $g = e^{2u} g_{S^2}$ on S^2 .*

More precise results in the spirit of Morse theory were obtained by Chang-Yang in [8], and later by Han [11], Chang-Gursky-Yang [5], and Chang-Liu [6]. In particular, these results extend Theorem 1.1 to the case of many local maxima. It is hoped that there is a condition on f which is both necessary and sufficient for the existence of a conformal metric having f as its Gauss curvature. However, in spite of much effort, so far no such condition has been found.

In [18], we partially resolve this question by showing that to a certain extent Theorem 1.1 is best possible; that is, we give examples of functions f having exactly two local maxima and one saddle point Q where $\Delta f(Q) < 0$ that cannot be realized as curvature functions of conformal metrics on S^2 .

We also give a new proof of Theorem 1.1 by analyzing the prescribed curvature flow, which seems to be the most natural approach. In fact, in the context of this flow many of the results in the references mentioned above and the analytic ideas behind them appear clearly motivated by geometry. Moreover, the prescribed curvature flow possesses a structure which is very similar to the Calabi and Ricci-Hamilton flows on S^2 that we studied in [17].

The key compactness result Lemma 3.1 may be of independent interest. In particular, our construction of examples for non-existence heavily relies on this result.

In the forthcoming paper [14] with Malchiodi, we carry over this approach to the analogous higher-dimensional evolution problem for prescribed Q -curvature on S^4 , giving rise to existence results analogous to Theorem 1.1, which improve the ones previously obtained by Brendle [4] by other methods.

For the “subcritical” case when the underlying manifold is not conformally equivalent to the sphere, a similar flow approach was introduced by Baird et al. [2] and, in the higher-dimensional case, by Brendle [3].

2. THE FLOW

For ease of exposition in the sequel we focus on Nirenberg’s problem on S^2 . Let $f \in C^\infty(S^2)$ be given with $f > 0$. Any metric g on S^2 conformal to the standard metric g_{S^2} may be represented as $g = e^{2u}g_{S^2}$ for some function u on S^2 . Given a metric $g_0 = e^{2u_0}g_{S^2}$ satisfying the condition

$$(2.3) \quad \text{vol}(S^2, g_0) = \int_{S^2} d\mu_{g_0} = 4\pi,$$

we evolve g_0 towards a metric g_∞ of Gauss curvature proportional to f through a family of metrics $g(t) = e^{2u(t)}g_{S^2}$, $t \geq 0$, by solving the flow equation

$$(2.4) \quad u_t = \frac{du}{dt} = \alpha f - K,$$

with initial data $g(0) = g_0$. Here $K = K_g$ is the Gauss curvature of $g = g(t)$; moreover, we determine $\alpha = \alpha(t)$ so that

$$(2.5) \quad \alpha \int_{S^2} f d\mu = 4\pi$$

for all $t \geq 0$, where $d\mu = d\mu_g = e^{2u}d\mu_{g_{S^2}}$. The Gauss-Bonnet theorem (1.1) then yields the equation

$$\frac{d}{dt} \left(\int_{S^2} d\mu \right) = 2 \int_{S^2} u_t d\mu = 2 \int_{S^2} (\alpha f - K) d\mu = 0,$$

and (2.3) implies the identity

$$(2.6) \quad \text{vol}(S^2, g) = \int_{S^2} d\mu = 4\pi$$

for all $t \geq 0$. In view of the Gauss equation

$$(2.7) \quad -\Delta_{g_{S^2}} u + 1 = K e^{2u}$$

equation (2.4) defines a nonlinear parabolic evolution equation for u .

Denote as

$$\bar{u} = \int_{S^2} u \, d\mu_{g_{S^2}} = \frac{1}{4\pi} \int_{S^2} u \, d\mu_{g_{S^2}},$$

the mean value of u , etc., and let

$$E(u) = \int_{S^2} (|\nabla u|_{g_{S^2}}^2 + 2u) \, d\mu_{g_{S^2}}$$

be the Liouville energy of g . Also define the functional

$$E_f(u) = E(u) - \log \left(\int_{S^2} f e^{2u} \, d\mu_{g_{S^2}} \right).$$

The flow (2.4) may be interpreted as the (negative) gradient flow for E_f .

Lemma 2.1. *For a smooth solution of (2.3) - (2.5) there holds*

$$\frac{d}{dt} E_f(u) = -2 \int_{S^2} |\alpha f - K|^2 \, d\mu \leq 0.$$

Since E_f is bounded from below, for a suitable sequence $t_l \rightarrow \infty$ ($l \rightarrow \infty$) with associated metrics $g_l = g(t_l)$, and letting $K_l = K_{g_l}$, we then obtain convergence

$$(2.8) \quad \int_{S^2} |K_l - \alpha(t_l) f|^2 \, d\mu_{g_l} \rightarrow 0 \quad (l \rightarrow \infty).$$

Provided that we also can show convergence of the associated sequence of metrics g_l to a limit metric g_∞ with Gauss curvature K_{g_∞} it follows that $K_{g_\infty} = \alpha f$ for some number $\alpha > 0$ and the rescaled metric αg_∞ will have curvature f .

Conversely, assuming that the given function f cannot be realized as the Gauss curvature of any conformal metric, the metrics $g(t)$ concentrate and become nearly spherical, as described below.

3. CONCENTRATION-COMPACTNESS

The following result is related to [7], Proposition A, [17], Theorem 3.1, or [9], but goes beyond these results as it allows a precise characterization of the microscopic concentration behavior of metrics.

Lemma 3.1. *Let (u_l) be a sequence of smooth functions on S^2 with associated metrics $g_l = e^{2u_l} g_{S^2}$, $l \in \mathbb{N}$. Suppose that $\text{vol}(S^2, g_l) = 4\pi$ and $\|K_{g_l} - K_\infty\|_{L^2(S^2, g_l)} \rightarrow 0$ as $l \rightarrow \infty$ for some smooth function $K_\infty > 0$ on S^2 . Also let $h_l = \Phi_l^* g_l = e^{2v_l} g_{S^2}$ be the associated sequence of normalized metrics as in Section 3.2. Then, either*

i) for a subsequence $l \rightarrow \infty$ we have $u_l \rightarrow u_\infty$ in $H^2(S^2)$, where $g_\infty = e^{2u_\infty} g_{S^2}$ has Gauss curvature K_∞ , or

ii) the metrics g_l become uniformly “round” and “concentrated” in the sense that for every sequence $l \rightarrow \infty$ there exist a subsequence, again denoted as (u_l) , and a point $Q \in S^2$ such that, as $l \rightarrow \infty$,

$$(3.9) \quad d\mu_{g_l} \rightarrow 4\pi \delta_Q$$

weakly in the sense of measures, while

$$(3.10) \quad h_l \rightarrow g_{S^2} \text{ in } H^2(S^2);$$

in particular, $K_{h_l} \rightarrow 1$ in $L^2(S^2)$. Moreover, in the latter case Φ_l weakly converges in $H^1(S^2)$ to the constant map $\Phi_\infty \equiv Q$.

As a consequence of Lemma 3.1, if the given function f cannot be realized as the Gauss curvature of any conformal metric, the flow (2.4) degenerates to a finite-dimensional pseudo-gradient flow for f on S^2 in the sense that the metrics $g(t)$ become more and more spherical and concentrate more and more around points $P(t) \in S^2$ that move in direction of increasing values of f . The dynamics then essentially is captured by the projection of the flow speed onto a three-dimensional space of eigenfunctions φ_i^g of Δ_g , $i = 1, 2, 3$, the generators of the group of conformal diffeomorphisms, governing the concentration scale of the evolving metrics and the gradient-like motion of the concentration points $P(t)$, respectively. Similar to Chang-Yang we show that this “shadow” flow may only accumulate at local maximum points of f or at saddle points Q where $\Delta f(Q) \leq 0$. Theorem 1.1 then follows.

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On the two-well problem with surface energy

SERGIO CONTI

In the theory of solid-solid phase transitions one minimizes functionals of the form

$$I_\varepsilon[u] = \int_\Omega \frac{1}{\varepsilon} W(\nabla u) + \varepsilon |\nabla^2 u|^2 dx$$

where $u : \Omega \subset \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $W : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$ behaves qualitatively as the squared distance from the set $K = SO(n)A \cup SO(n)B$. The matrices A and B characterize the two admissible phases, and we are interested in the case where they are compatible, in the sense that $\text{rank}(A - B) = 1$.

For small ε one expects I_ε to reduce to a sharp-interface model. In this talk several results in this direction have been presented, under various simplifying assumptions on K and W . Precisely, it has been shown that I_ε converges, in the sense of Gamma convergence, to the functional

$$I_0(u) = \begin{cases} \int_{J\nabla u} k(\nu) d\mathcal{H}^{n-1} & \text{if } \nabla u \in BV(\Omega, K) \\ \infty & \text{else,} \end{cases}$$

where $J\nabla u$ is the jump set of ∇u , in the following three cases:

- (1) If K is replaced by $K' = \{A, B\}$, which is composed of only two matrices (joint work with I. Fonseca and G. Leoni [?])
- (2) If $n = 2$ and one linearizes the set of rotations $SO(2)$, i.e. K is replaced by $K'' = \{A + \omega, B + \omega : \omega = -\omega^T\}$, and Ω is star-shaped (joint work with B. Schweizer [?])
- (3) If $n = 2$ and K is the full set $K = SO(2)A \cup SO(2)B$, again with Ω star-shaped (joint work with B. Schweizer [?]).

The third result is based on an optimal $H^{1/2}$ -rigidity estimate for low-energy functions. The same rigidity argument permits to show that for functions with small surface energy the two-well energy controls the one-well one, in L^1 and upon taking a subdomain. Precisely, if $u : \Omega \rightarrow \mathbb{R}^2$ satisfies $\int |\nabla^2 u| \leq c$, then

$$\min_{J \in \{A, B\}} \|\text{dist}(\nabla u, SO(2)J)\|_{L^1(\Omega')} \leq c \|\text{dist}(\nabla u, K)\|_{L^1(\Omega)}$$

for any connected $\Omega' \subset\subset \Omega$, with constants depending on A, B, Ω and Ω' (joint work with B. Schweizer, [?]). This improves a previous result by A. Lorent [?] who obtained the first quantitative two-well rigidity estimate, for the case that u is bilipschitz and $\det A = \det B$. Precisely, he obtained $\min_J \|\text{dist}(\nabla u, SO(2)J)\|_{L^1(\Omega')} \leq c \|\text{dist}(\nabla u, K)\|_{L^1(\Omega)}^{1/800}$. The present result gives the optimal exponent.

Crystallisation in two dimensions

FLORIAN THEIL

Why do many solids form crystals? In order to shed light on this classical question we consider $N \in \mathbb{N}$ particles in \mathbb{R}^d , $d \in \{1, 2, 3\}$ and study the asymptotic behavior of ground states of the following pair-interaction energy

$$E(y) = \sum_{\{x, x'\} \subset X} V(|y(x) - y(x')|)$$

as N tends to infinity. Here X is a finite set, $\#X = N$, $y : X \rightarrow \mathbb{R}^d$ encodes the positions of N particles and $V : [0, \infty) \rightarrow \mathbb{R}$ is a fixed interaction potential.

Theorem A. (*Asymptotic behaviour of the ground state energy per particle*)

Let $d = 2$. There exists a constant $a > 0$ such that for all $V \in C^2(0, \infty)$ with the properties $V(1) = -1$, $\lim_{r \rightarrow \infty} V(r) = 0$ and

$$\begin{aligned} V(r) &\geq \frac{1}{a} \text{ and for all } r \in [0, 1 - a], \\ V''(r) &\geq 1 \text{ and for all } r \in (1 - a, 1 + a), \\ V(r) &\geq -\frac{1}{2} \text{ and for all } r \in [1 + a, \sqrt{2}], \\ V''(r) &\leq ar^{-5} \text{ and for all } r < \sqrt{2}, \end{aligned}$$

the ground state energy has the following asymptotic behavior

$$\lim_{N \rightarrow \infty} \frac{1}{N} \min_y E(y) = 3 \min_r V_R(r) = 3V_R(r_*) = 3E_*.$$

The renormalized potential V_R , which is defined by

$$V_R(r) = \frac{1}{6} \sum_{k \in \mathbb{Z}^2 \setminus \{0\}} V\left(r\sqrt{k_1^2 + k_1k_2 + k_2^2}\right),$$

is the interaction energy between a single particle and a homogeneously stretched copy of the hexagonal lattice

$$A_2 = \left\{ \frac{1}{2} \begin{pmatrix} 2 & 1 \\ 0 & \sqrt{3} \end{pmatrix} k \mid k \in \mathbb{Z}^2 \right\} \subset \mathbb{R}^2.$$

In particular the result implies that the ground state energy is asymptotically proportional to the number of particles, not the number of terms in E .

Theorem B. (*Ground states*)

Let the assumptions of Theorem A be satisfied, $\mathcal{A} \subset A_2$ be an arbitrary bounded subset and y_{\min} be a ground state of the modified energy

$$\sum_{\substack{x \in \mathcal{A} \\ x' \in A_2}} V(|y(x) - y(x')|)$$

subject to the constraint $y(x) = r_*x$ for all $x \in A_2 \setminus \mathcal{A}$. Then $\{y(x) \mid x \in A_2\} = r_*A_2$.

Previously Radin obtained in [1] similar results for a specific choice of V .

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Compact constant Mean Curvature Surfaces revisited

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The theory of constant mean curvature surfaces in Euclidean space has been the object of intensive study in the past years. In the case of complete noncompact constant mean curvature surfaces, the moduli space of such surfaces is now fairly well understood (at least in the genus 0 case) [9], [7], [8] and many technics have been developed to produce examples of such surfaces [6], [3], [10], [12].

By contrast, the set of compact constant mean curvature surfaces is not so well understood. In the early 80's, H. Wente has constructed the first examples of genus 1 constant mean curvature surfaces [15]. These genus 1 surfaces have then been thoughtfully studied by U. Pinkall and I. Sterling [13]. Examples of compact constant mean curvature surface of higher genus are due to N. Kapouleas. In the genus 2 case [5], these surfaces are obtained by "fusing" Wente tori while in the case where the genus is greater than or equal to 3, these surfaces are obtained by connecting together large number of mutually tangent unit spheres, using small catenoid necks [4].

In a joint work with M. Jleli, we explain how the current knowledge on the set of *complete noncompact* constant mean curvature surfaces can be exploited to produce new examples of compact constant mean curvature surfaces of genus greater than or equal to 3.

Our construction is based on tools which have been developed for the understanding of complete noncompact constant mean curvature surfaces. This construction can be described as follows :

- (1) Since the first construction by N. Kapouleas [3], many constructions of *complete noncompact* constant mean curvature surfaces have then been developed [6], [3], [10], [11], [12]. These constructions provide an important source of examples of *complete noncompact* constant mean curvature surfaces the geometry of whose ends is prescribed.
- (2) Most of the above mentioned constructions are quite flexible and one can arrange so that the ends of these surfaces can be "plugged" together to produce sequences (indexed by a discreet parameter $n \in \mathbb{N}$) of *compact* surfaces which have mean curvature equal to 1 except in finitely many annular regions where their mean curvature can be estimated by $1 + O(e^{-\gamma^n})$ for some $\gamma > 0$. This is essentially the "end-to-end" construction which was developed by J. Ratzkin [14] to connect (and produce) complete noncompact constant mean curvature surfaces along their ends.

- (3) Next, one studies the mapping properties of the Jacobi operator about this (almost) constant mean curvature surface. To perform this analysis, we rely on the fact that parametrices for the Jacobi operators on each complete noncompact summand have been obtained in the "moduli space theory" developed by R. Kusner, R. Mazzeo and D. Pollack [9]. We explain how these can be glued together. This construction requires a precise understanding of the set of Jacobi fields on each summand.
- (4) Finally, it remains to use a standard perturbation argument to produce sequences of compact constant mean curvature surfaces of arbitrary genus, greater than or equal to 3.

We believe that the main advantage of our construction versus the one developed by N. Kapouleas is that it is technically simple (once the above mentioned results on complete noncompact surfaces are understood !), paralleling the fact that the end-to-end construction of J. Ratzkin is simpler than the previous constructions of complete noncompact surfaces. We obtain a very precise description of the surfaces we produce (the perturbation of the approximate surface is an exponentially decreasing function of the diameter of the surface constructed). In particular, our construction sheds light on the structure of the set of compact constant mean curvature surfaces, showing that these surfaces are isolated (modulo the action of rigid motions). Though this is probably a minor point, the example of compact constant mean curvature surfaces we obtain are geometrically different from the one obtained by N. Kapouleas (roughly speaking all the surfaces constructed by N. Kapouleas have close to sequences of unit spheres linked by small catenoids and hence have small injectivity radius while our examples do not necessarily have small necks and hence have injectivity radius uniformly bounded from below).

Maybe a more important issue is the fact that our construction points out interesting directions toward which the theory of complete noncompact constant mean curvature surfaces should be developed to understand the set of compact constant mean curvature surfaces. In the previous constructions some properties of complete noncompact constant mean curvature surfaces have been neglected and turn out to be extremely important. This is for example the case of the notion of "nondegeneracy" and the notion of "regular end" (both turn out to be also important in the construction of J. Ratzkin). Final remark, our construction generalizes in any dimension [1].

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On solutions of the relative isoperimetric problem

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A solution of the isoperimetric problem (or partitioning problem) relative to a given set $\Omega \subset \mathbb{R}^3$ is a subset E of Ω with prescribed volume $|E| = V \in (0, |\Omega|)$ and minimal area $\int_{\Omega} |D\chi_E| = A(V)$. If Ω is convex, then the function $A(V)^{3/2}$ is concave. At the beginning of the talk we prove this simple fact and observe some geometric consequences; in particular, a convex set separates always better than the halfspace. For related results see [5] and [2].

In the main part of the talk which is joint work with W. Bürger (Freiburg), we discuss an approach constructing minimizers within the class of disk-type surfaces. This is motivated by an open conjecture by A. Ros [4] saying that, for Ω convex, the boundary of the minimizer within the class of Cacciopoli sets should actually be a disk. We work in the class of surfaces parametrized on the disk, possibly with selfintersections, and do not treat $\partial\Omega$ as an obstacle. The volume is counted with multiplicities. For general sets Ω with smooth boundary we construct a minimizer within the class of surfaces which are unions of finitely many disks. For Ω convex, we conjecture that this solution is a single disk.

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Quasistatic evolution of damage

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(joint work with C. Francfort)

We construct a quasi-static evolution for a variational model for damage proposed by Francfort and Marigo, [3]. More precisely given an elastic body and an external loading $f(t)$ parametrized by time, we look for a function $u(x, t)$ representing the deformation of the body Ω in the damaging process. Moreover, we would also like to determine a time-parametrized family of increasing subsets of Ω which represents the evolving damaged region. This is done through a time-discretization procedure.

The two states, undamaged and damaged, are given by two elastic well-ordered tensor, A_s and A_w , and the energy is given by

$$\int_{\Omega} W(e(u)) dx - \int_{\Omega} f u dx,$$

where $e(u) = \frac{\nabla u + \nabla u^T}{2}$ is the symmetrized gradient and

$$W(\varepsilon) = \min \left\{ \frac{1}{2} A_s \varepsilon \varepsilon, \frac{1}{2} A_w \varepsilon \varepsilon + K \right\}.$$

This energy density is not quasi-convex; thus in the minimization procedure we expect microstructure, in other words we expect a relaxation phenomenon. The quasi-convex envelope of W can be represented as follows

$$QW(\varepsilon) = \min_{\theta \in [0,1]} \min_{A \in G_{\theta}(A_s, A_w)} \left\{ \frac{1}{2} A_s \varepsilon \varepsilon + K \theta \right\},$$

where $G_{\theta}(A_s, A_w)$ is the G -closure of A_s and A_w mixed with volume fraction θ and $1 - \theta$. Starting from this formula we construct a discrete time evolution which accounts for the constraint of irreversibility of the damage region, prove convergence and regularity of the limit.

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Refined Jacobian estimates

ROBERT J. JERRARD

A typical Jacobian estimate for Ginzburg Landau functionals has the form

$$(0.1) \quad \|Ju\|_{(C_c^{0,\alpha}(U))^*} \leq C \left(\varepsilon^\beta + \frac{1}{|\ln \varepsilon|} \int e_\varepsilon(u) \, dx \right). \quad \text{for all } u \in H^1(U; \mathbb{R}^2)$$

where U is a bounded open subset of \mathbb{R}^n ; $Ju = \sum_{i < j} \det(u_{x_i}, u_{x_j}) \, dx^i \wedge dx^j$ is the pullback by u of the standard volume form on \mathbb{R}^2 ; and $e_\varepsilon(u)$ is the Ginzburg-Landau energy density

$$e_\varepsilon(u) = \frac{1}{2} |\nabla u|^2 + \frac{1}{4\varepsilon^2} (|u|^2 - 1)^2.$$

Here the constant C may depend on the domain U and on the parameter α in the norm on the right-hand side, but is uniform for $\varepsilon \in (0, 1/2]$. Estimates in this spirit have been established in [8], [1], [12] for example. Such estimates are useful when $\varepsilon \ll 1$ due to the factor of $|\ln \varepsilon|^{-1}$ on the right-hand side.

Some applications of Jacobian estimates include the following:

1. A refinement of (0.1), taking into account boundary values of u , was proved by Bethuel, Bourgain, Brezis, and Orlandi [2], who applied it to establish uniform $W^{1,p}$ estimates, $p < n/n - 1$, for solutions u_ε of the equation

$$(0.2) \quad -\Delta u_\varepsilon + \frac{1}{\varepsilon^2} (|u_\varepsilon|^2 - 1)u_\varepsilon = 0$$

in a bounded, smooth domain $U \subset \mathbb{R}^n$ with the boundary condition

$$u = g \in H^{1/2}(\partial U; S^1) \text{ on } \partial U$$

and satisfying the natural energy bound $\int_U e_\varepsilon(u_\varepsilon) \leq M_0 |\ln \varepsilon|$. Very crudely, the argument rests on the fact that one can decompose ∇u_ε into a number of pieces, one of which is essentially Ju_ε , and with all the others controlled in some way by the equation (0.2). This general approach has proved quite robust, and has yielded good estimates for a number of related equations, including Ginzburg-Landau heat flow [4] for example.

2. Jacobian-type estimates play a key role in results characterizing the Γ -limit of Ginzburg-Landau functionals, see [1]. These results have been used in [11] to prove the existence of certain solutions of (0.2). Similar results have been established for related, more complicated equations describing superconductors [7] and Bose-Einstein condensates [6].

3. An analysis of vortex dynamics in solutions of the equation

$$(0.3) \quad i\partial_t u_\varepsilon - \Delta u_\varepsilon + \frac{1}{e^2} (|u_\varepsilon|^2 - 1)u_\varepsilon = 0, \quad u_\varepsilon \in C([0, T]; H^1(U; \mathbb{C}))$$

in the limit $\varepsilon \rightarrow 0$ was carried out by [5] and [10] for $U \subset \mathbb{R}^2$ with suitable assumptions on the initial and boundary data. Jacobian-type estimates and related Γ -convergence results are used in these proofs. The relevance of Jacobians for this problem stems from 2 facts. First, limits of Jacobians can be used to identify asymptotic vortex locations. More precisely, Γ -limit type results show

that, under hypotheses satisfied by sequences of solutions of (0.3), sequences $Ju_\varepsilon(\cdot, t)$ are precompact in certain weak norms, and any limit must have the form $\sum \pi d_i \delta_{a_i} dx^1 \wedge dx^2$. These points a_i are interpreted as being limiting vortex positions.

Second, for a solution of (0.3), the Jacobian satisfies the identity

$$\partial_t Ju_\varepsilon = \mathbb{J}_{ij} \operatorname{Re}(u_{\varepsilon, x_j} \bar{u}_{\varepsilon, x_k})_{x_i x_k}$$

where \mathbb{J} is a 2×2 symplectic matrix and Re indicates the real part. (This is simply the curl of the equation for conservation of momentum for (0.3).) This means that one can control time evolution of the Jacobian, and hence of the vortex locations, by controlling a single space derivative of u_ε .

The refined Jacobian estimates stated below are motivated in part by the goal of establishing results about vortex dynamics for (0.3) that would be valid for fixed $0 < \varepsilon \ll 1$, rather than only in the limit $\varepsilon \rightarrow 0$.

Theorem 0.1 ([9]). *Let U_r denote the open ball $\{x \in \mathbb{R}^2 : |x| < r\}$. Assume that $u \in H^1(U_r; \mathbb{C})$ and that*

$$(0.4) \quad \|Ju - \pi\delta_0\|_{\dot{W}^{-1,1}(U_r)} < \frac{\pi}{200}r$$

Then there exists $\xi \in U_{r/2}$ such that if we write

$$(0.5) \quad K_0 = \int_{U_r} e_\varepsilon(u) dx - \pi \ln \frac{r}{\varepsilon}.$$

then

$$(0.6) \quad \|Ju - \pi\delta_\xi\|_{\dot{W}^{-1,1}(U_r)} \leq \varepsilon \sqrt{\ln(r/\varepsilon)} C(1 + K_0)^2 e^{K_0/\pi}$$

C is independent of $\varepsilon \in (0, r/2]$ and of K_0 .

The conclusion (0.6) asserts, heuristically, that the Jacobian Ju is localized down to length scales of order $\varepsilon \sqrt{\ln(r/\varepsilon)}$, and thus that it can be used to determine vortex locations to this order of precision. This estimate is close to sharp in that for fixed K_0 , one can construct functions u_ε satisfying (0.4), (0.5) and $\|Ju - \pi\delta_\xi\|_{\dot{W}^{-1,1}(U_r)} > C^{-1}\varepsilon \sqrt{\ln(r/\varepsilon)} e^{K_0/\pi}$. Theorem 0.1 can be used to show that, under hypotheses that are preserved (at least for short times) by the evolution equation (0.3), an estimate of the form

$$\|Ju - \pi \sum_{i=1}^n d_i \delta_{\xi_i}\|_{\dot{W}^{-1,1}(U_r)} \leq C\varepsilon \sqrt{\ln(r/\varepsilon)}$$

Thus one can hope to use the Jacobian to locate vortices in solutions of (0.3) for $0 < \varepsilon \ll 1$ with great precision. This is a starting point for further work.

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Finite differential inclusion and elliptic regularity

BERND KIRCHHEIM

(joint work with A.Pratelli)

We discuss ongoing attempts extend the class of counterexamples to elliptic regularity as it was introduced in [4]. In particular, in [2] the question was investigated for which specific equations the corresponding first order partial differential inclusion allows solutions. It turned out, however that adding convex terms to an elliptic system that originally allowed no irregular solutions constructed by convex integration may lead to unexpected difficulties when one has to decide if such solutions can still be excluded.

It could be shown that the original T_4 -configuration which could be embedded into the differential inclusion

$$\mathcal{K}_F = \left\{ \begin{pmatrix} X \\ DF(X)J \end{pmatrix} ; X \in \mathbb{R}^{2 \times 2} \right\} \subset \mathbb{R}^{4 \times 2},$$

corresponding to the Euler-Lagrange equation

$$\operatorname{div} DF(\nabla u) = 0$$

for suitable quasiconvex $F : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}$ has now to be replaced by more complicated configurations.

Indeed, whereas Székelyhidi (see [5]) managed to utilise a T_5 -configuration for a basically randomly selected polyconvex energy F , in [2] we could show that for the (above mentioned) energy

$$F(X) = \varepsilon |X|^2 / 2 + \det(X)^2$$

there are no finitely supported laminates in \mathcal{K}_F whose first projection lives in the diagonal matrices. Unfortunately, the existence of more diffuse laminates remains open, but it is known that simple approximation arguments are not available.

Here we present a result pointing in the opposite direction, we show that using and substantially refining an idea from [1] we can avoid even the “diffusive” perturbation process used in [4] and [5]. It is indeed possible to obtain nowhere C^1 -Lipschitz solutions u of $\operatorname{div} DF(\nabla u) = 0$ where F is polyconvex but u has only finitely many different gradients ([3]). Recent progress in combinatorial approaches to the study of rank-one convexity supports the hope that the investigation of such finite differential inclusions can lead to more conclusive existence results.

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