Mathematisches Forschungsinstitut Oberwolfach

Report No. 19/2001

Phasenübergänge

April 29th – May 5th, 2001

This meeting was organized by Hans Wilhelm Alt (Bonn), Stephan Luckhaus (Leipzig), Errico Presutti (Roma II) and Ekhard K. H. Salje (Cambridge). It focussed on a variety of mathematical models for phase transitions and their applications, bringing together mathematicians working on areas as statistical mechanics, stochastics, mathematical physics, PDE and numerical analysis with engineers and physicists.

The aim of the meeting was to create interaction between researchers from these different areas. Many lively discussions after the talks showed that at least a first step in this direction has been made. The talks given at the meeting covered the following areas:

- The approach from statistical mechanics/stochastics: Phase transitions as loss of regularity of thermodynamic potentials and loss of symmetry of Gibbs measures, moreover large deviations, metastability and aging and optimal shape questions for phase fractions.
- The deterministic passage from atomistic or mesoscale models to sharp interface models in the equilibrium case, using e.g. Γ-convergence and tools from geometric measure theory.
- Evolution equations describing the behaviour of systems undergoing phase transitions on different scales, motion of phase boundaries and the difficulties of possible non-separation of scales or lattice effects.
- Numerical methods and models aimed at applications in industry.

Edited by Nicolas Dirr, Leipzig

Abstracts

Asymptotic limits of local and nonlocal models in phase transitions

Giovanni Bellettini (Univ. of Roma "Tor Vergata")

In this talk I made an overwiew of some recent results on the asymptotic limits of (possibly anisotropic) Allen-Cahn type functionals arising in phase transitions and of their nonlocal counterpart, under the ferromagnetic assumption (i.e., when the interaction potential J is nonnegative). I have discussed the relations between the gradient flow of the limit energy and the equation obtained as the limit of the gradient flows of the Euler Lagrange equations of the approximating functionals, both in the local case and in the nonlocal case. This correspondence is non trivial, because the functionals at hand are far from being convex. In the nonlocal case it turns out that the surface tension (i.e., the integrand of the limit functional) is strictly convex and smooth. Understanding whether it is possible to get a faceted surface tension by relaxing the assumptions on J is an open question. Finally, I briefly discussed the asymptotic limits of the elliptic problems associated to the approximating functionals (only in the local case) and the connection with the so called prescribed curvature problem.

Phase transitions and convection

Thomas Blesgen, Universität Leipzig

Let $\Omega \subset \mathbb{R}^d$, $1 \leq d \leq 3$ be a bounded domain with Lipschitz boundary. For $0 < D \leq \infty$ let $\Omega_D := \Omega \times (0, D)$ and $\varrho : \Omega_D \to \mathbb{R}^+$ denote the (averaged) density of the fluid, $e : \Omega_D \to \mathbb{R}^+$ the internal energy, $v : \Omega_D \to \mathbb{R}^d$ the velocity field of the fluid. Governed by a phase parameter $\chi : \Omega_D \to [0, 1]$, two phases may exist in Ω. For the potential energy density $E_{\rm pot}$ of the system, $E_{\rm pot} = \chi E_{\rm pot,1} + (1 - \chi) E_{\rm pot,2}$ is postulated. Similar relationships are assumed for the entropy density S and the Gibbs free energy density G. The internal energy e is obtained after adding the kinetic energy:

$$e = e_{\rm pot} + \frac{\varrho}{2} |v|^2.$$

After introducing a mixing entropy, S obeys the formula

$$\begin{aligned} S &= \chi S_1 + (1 - \chi) S_2 - W(\chi) - \frac{\delta}{2} |\nabla \chi|^2, \\ W(\chi) &:= \chi \ln \chi + (1 - \chi) \ln(1 - \chi) - \frac{1}{2} \chi^2. \end{aligned}$$

For δ, $\varepsilon > 0$ and the inlet R_I, the outlet R_O of Ω we introduce the system:

$$\begin{aligned} \partial_t \varrho &= -\mathrm{div}(\varrho v), \\ \partial_t (\varrho v) &= -\mathrm{div}(\varrho v \otimes v + \delta \varrho T \nabla \chi \otimes \nabla \chi) + \mathrm{div}(\tau) - \nabla p, \\ \partial_t e &= \mathrm{div}(L \nabla T - (e - \Gamma) v), \\ \varepsilon \, \partial_t \chi &= -W'(\chi) - \frac{1}{T} (G_1 - G_2)(\rho, T) + \frac{\delta}{\varrho} \mathrm{div}(\varrho \nabla \chi) - \varepsilon v \cdot \nabla \chi \end{aligned}$$

in Ω *with the given initial values*

$$(\varrho, \varrho v, e, \chi)(\cdot, 0) = (\varrho_0, \varrho_0 v_0, e_0, \chi_0) \qquad \text{in } \Omega$$

and the boundary values

$$\chi = \chi_r, \quad v = v_r, \quad T = T_r \quad on\ \partial\Omega, \quad \varrho = \varrho_I \quad on\ R_I.$$

It can be shown that for the resulting model the second law of thermodynamics is valid. Global existence of a solution holds for instance if the system is assumed to be incompressible.

Aging in the random energy model

Anton Bovier, WIAS Berlin

(joint work with G. Ben Arous and V. Gayrard)

The concept of "aging" is a rather new paradigm for the description of the asymptotics of dynamical behaviour in complex systems, and in particular large random or "glassy" systems that is heavily studied in the physics literature. In general terms, it is characteristic of systems that, on the time scale on which they are observed, do not converge to equilibrium exponentially fast and whose "age" can therefore be deduced from the observation of the system at a given time t. A general indicator for aging is e.g. a autocorrelation function $C(t, t+s)$ that is a function of s/t only.

One of the simplest models that is expected to show aging in its dynamics is the random energy model (REM) under Glauber dynamics. In spite of its simplicity, even in the physics literature, no real results on the dynamics of this model are available; however, Bouchaud introduced several years ago that is known as the "REM-like trap model" which permits exact computations of the autocorrelation functions and which indeed shows very nicely the aging phenomenon. In this talk I explain these ideas in some detail, and present a rigorous derivation of the aging dynamics in the full REM for a special choice of the Glauber dynamics. It is found that one may define a properly rescaled autocorrelation function representing the probability that the process moves from one of the most low-lying states to another one between times tC_N and $(t+s)C_N$ has exactly the same asymptotic behaviour as the corresponding autocorrelation function in the REM like trap model. The proof relies on the analysis of a system of renewal equations whose kernel is defined in terms of the distribution of the transition times between sites σ and σ' and depends on sharp estimates of these quantities that use methods of two recent papers (A. Bovier, M. Eckhoff, V. Gayrard and M. Klein, *"Metastability in stochastic dynamics of disordered mean-field models"*, Prob. Theor. Rel. Fields 119, 99-161(2001), and *"Metastability and low-lying spectra in reversible Markov chains",* WIAS-preprint 601 (2000), submitted to Commun. Math. Phys.)

Proper ferroelastic phase transitions in thin epitaxial films with symmetry-conserving and symmetry-breaking misfit strains

A.M. Bratkovsky, Hewlett-Packard Laboratories, Palo Alto, USA

(joint work with A.P. Levanyuk)

We study how the ferroelastic domain structure sets in an epitaxial film of a material with a second order proper ferroelastic transition. The domain structures considered are similar to either $a_1|a_2|a_1|a_2$ or c/a structures in perovskite ferroelectrics. If the "extrinsic" misfit strain, not associated with the transition, does not break the symmetry of the high-temperature phase, the phase transtion in the film occurs at somewhat lower temperature compared to the bulk. The loss of stability then occurs with respect to a sinusoidal strain

wave, which evolves into the domain structure of basically the same geometry and with approximately the same period. In the presence of the symmetry-breaking component of the misfit strain ("extrinsic" misfit) the character of the phase transion is qualitatively different. In this case this is a topological transition between single-domain and multi-domain states, which starts from a low density of the domain walls. There is no critical thickness, below which the domain structure cannot exist, when the "extrinsic" misfit is zero and the domains are of equal width. At the boundary of polydomain-monodomain transition the period of the pattern diverges, as does the dynamic stiffness of the domain structure. It is unlikely, therefore, that one can achieve a softness of the dielectric response of the c/a elastic domains in ferroelectric-ferroelastic thin films.

Surface structure of domain walls

S. Conti (MPI Leipzig)
(joint work with E.K.H. Salje (Cambridge))

Domain walls offer a rare opportunity to selectivly dope two-dimensional sections in the bulk of crystalline materials. The enhanced chemical reactivity of the elastically strained region around the domain wall has been demonstrated experimentally, and has been used to form two-dimensional superconducting regions in an insulating matrix. The process of selective doping is in large part controlled by the elastic strains present in the material, and by their interaction with surface relaxation.

We have developed a model based on continuum elasticity and energy minimization for the study of the behaviour of ferroelastic domain walls close to a flat surface. The model predicts a double-peak structure in the squared elastic strain, which is directly related to the chemical reactivity, around the intersection of the domain wall with the surface. We also compute the height profile, which is in principle measurable with AFM, and the strain distribution in the bulk. Our results are in good agreement with previous atomistic simulations which had required much bigger computational effort.

Probabilistic models for Stefan problems

Nicolas Dirr, Leipzig
(joint work with S. Luckhaus)

A Stefan problem is a model for the evolution of phase boundaries coupled to a diffusion equation. Motivated by the fact that weak solutions for Stefan problems with surface tension do in general not converge to weak solutions of Stefan problems without surface tension ("mushy phase") we discuss whether the formation of a mushy phase can be explained as large deviation of a stochastic process converging to a Stefan problem with small but finite surface tension.

We present a stochastic lattice model where the spin variables flip with rates depending both on a Kac-potential type interaction with the neighbouring spins and on an intercation with a field, which plays the role of the external field in ferromagnetics but evolves by a diffusion equation with a forcing depending on the spins ("latent heat"). The mesoscopic limit is a nonlocal analogue of the phase field equations.

However a simpler toy model suggests that large deviations from such models cannot create a mushy phase region.

Industrial needs versus cababilities of phase field models

Wolfgang Dreyer, WIAS Berlin

We study phase field models which are cabable to simulate the coarsening process observed during thermo-mechanical treatment of binary tin-lead solders and of single crystal galliumarsenid. More specifically, the analysis is based on a continuum theory which relies in many aspects on an atomistic point of view.

We give an atomistic interpretation of the Gibbs free energy of a binary alloy. Deviations from the classical theory as outlined in the seminal paper by Cahn and Hilliard are discussed, various other higher gradient terms for the extended diffusion flux are derived, and their influence on microstructural development is assesed quantitatively.

Fourier transforms are used for the numerical treatment of the thermo-elastic as well as of the diffusion problem encountered during phase separation in these alloys. The numerical computation of local stresses, strains and the concentration fields of the constituents are performed in a representative volume element. Special interest is devoted to the coupling of the mechanical and the thermodynamical problem.

A two-scale phase field model for liquid-solid phase transitions with dendritic microstructure

Christof Eck, Erlangen

A two-scale model describing solidification processes with dendritic microstructure is presented. The model is based on a simple phase field model for binary material proposed by Caginalp and Xie. A periodic initial distribution of solid kernels with mutual distance ε is assumed, the interface thickness parameter and the solute diffusivity are scaled proportional to ε and ε^2, respectively. Then the limit problem for $\varepsilon \to 0$ is computed by a formal asymptotic expansion.

The result is a two scale model consisting of a global averaged energy transport equation given on the macroscopic domain Ω and, at each point $x \in \Omega$, of a local cell problem describing the evolution of single crystals and the microscopic solute distribution.

The homogenization limit is justified by an error estimate comparing the solution of the two scale model to that of the original problem with scale ε.

Higher Order Variational Problems

Irene Fonseca, Carnegie Mellon University, Pittsburgh, USA

Higher order variational theories are relevant in the study of elasto-plastic materials (with micro cracks) and image segmentation in computer vision (the Blake Zisserman model). In order to illustrate the difficulties introduced by second order derivatives in a variational context, we will address lower semicontinuity and phase transitions for multiple integrals involving second order derivatives.

I. Lower Semicontinuity Properties for Multiple Integrals in $W^{k,1}(\Omega;\mathbb{R}^d)$

(work in collaboration with Giovanni Leoni, Jan Malý and Roberto Paroni)

Lower semicontinuity properties of multiple-integrals

$$u \in W^{k,1}(\Omega;\mathbb{R}^d) \mapsto \int_\Omega f(x, u(x), \cdots, \nabla^k u(x))\, dx$$

are studied when f grows at most linearly with respect to the highest order derivative, $\nabla^k u$, and admissible $W^{k,1}(\Omega;\mathbb{R}^d)$ sequences converge strongly in $W^{k-1,1}(\Omega;\mathbb{R}^d)$. Here Ω is an open, bounded subset of $\mathbb{R}^N$, with $N \geq 1$, and $k, d \in \mathbb{N}$, $1 \leq p \leq \infty$.

When $k = 1$ the scalar case $d = 1$ has been extensively treated, while the vectorial case $d > 1$ was first studied by Fonseca and Müller and by Ambrosio and Dal Maso with respect to strong convergence in $L^1(\Omega;\mathbb{R}^d)$. When $k > 1$ and f depends in an intrinsic way on the lower order derivatives then $1 -$ *quasiconvexity* and $k -$ *polyconvexity* still provide lowersemicontinuity under appropriate growth conditions, but the genuine notion of k-quasiconvexity (although suitable for integrands such as $f(x, u(x), \cdots, \nabla^k u(x)) = h(x)g(\nabla^k u(x)))$ escapes our analysis. The approach in Fonseca and Müller is based on blow–up and truncation methods. Their main drawback lies in the fact that they cannot be easily extended to truncate gradients or higher order derivatives. One example was provided where in $(0,1)^N$, $N \geq 3$, we construct a sequence $u_n \in W^{2,2}$, $u_n \to 0$ in L^1, $\sup_n ||\Delta u_n||_1 < +\infty$, such that for some nonnegative smooth function h one has

$$\limsup_n \int_{(0,1)^3} h(u_n)(1 - \Lambda u_n)^+ < h(0).$$

This is in contrast with the case $k = 1$ which ensures that if $u_n \in W^{1,1}$ are such that $u_n \to u$ in L^1, $u \in BV$, anf if g is a nonnegative, convex function, then

$$\liminf_n \int_\Omega h(u_n)g(\nabla u_n) \geq \int_\Omega h(u)g(\nabla u).$$

II. Hessian Theory of Phase Transitions

(work in collaboration with Sergio Conti and Giovanni Leoni)

In the mid-80's the analysis of phase transitions for mixtures of two or more non-interacting fluids was successfully undertaken within the Van der Waals-Cahn-Hilliard gradient theory of phase transitions and modeled variationally through a family of singularly perturbed problems

$$J_\varepsilon(u;\Omega) := \int_\Omega \frac{1}{\varepsilon} W(u) + \varepsilon |\nabla u|^2 \, dx$$

where W is a nonnegative double-well potential with $\{W = 0\} = \{a, b\}$, and usually $u : \Omega \to \mathbb{R}$ has constrained average (corresponding to fixed volume fractions of each of the two constituents). The singular perturbations provide a selection criterion : minimizers of J_ε $\Gamma(L^1)$-converge to a minimizer of a minimal surface problem, namely

$$J(u;\Omega) := \begin{cases} K \operatorname{Per}_\Omega(u) & \text{if } u \in BV(\Omega;\{a,b\}), \\ +\infty & \text{otherwise,} \end{cases}$$

where the interfacial energy density is $K := 2\int_a^b \sqrt{W(s)}\, ds$. Generalizations to the case where W admits a curve of minima, multiple minima, or u takes vector values have been explored since by Bouchitté, Kohn and Sternberg, Baldo, Fonseca and Tartar, Barroso and Fonseca, among others. Higher order singular perturbations of nonconvex, multiple-well variational problems may be found in gradient strain theories in plasticity, ferromagnetics, and other areas of materials science and engineering, where J_ε now becomes

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

The characterization of the Γ-limit for this family has defied the analysis for over 10 years now. Partial results have been obtained since (e.g. Fonseca and Mantegazza), and in the two-dimensional case when W vanishes on the unit circle (one well and frame indifferent)

the problem reduces to the so-called eikonal functional which arises in the study of liquid crystals as well as in blistering of delaminated thin films (De Simone, Kohn, Müller and Otto, Aviles and Giga, Ambrosio, DeLellis and Mantegazza, Gioia and Ortiz, Jin and Kohn).

Assume that $\{W = 0\} = \{A, B\}$ where $\operatorname{rank}(A - B) = 1$. Under hypotheses satisfied by the prototype model $W(\xi) = \min\{|\xi - A|^2, |\xi - B|^2\}$, we show that there exists a constant K such that I_ε $\Gamma(L^1)$-converges to

$$I(u;\Omega) := \begin{cases} K \operatorname{Per}_\Omega(S(\nabla u)) & \text{if } u \in W^{1,1}(\Omega;\mathbb{R}^d), \nabla u \in BV(\Omega;\{A,B\}), \\ +\infty & \text{otherwise.} \end{cases}$$

A Waiting Time Phenomenon for the Thin Film Equation

Günther Grün, University of Bonn

(joint work with R. Dal Passo and L. Giacomelli, Roma)

The surface tension driven flow of thin films of viscous liquid spreading on a plane surface can be described by an evolution equation for the film height. This is accomplished by lubrication approximation, and the resulting equation is fourth order degenerate parabolic. For the model problem

$$h_t + \operatorname{div}(h^n \nabla \Delta h) = 0,$$

we prove the occurrence of a waiting time phenomenon provided initial data are sufficiently smooth. In space dimensions less or equal to three, we identify a general criterion on the growth of initial data near the free boundary which guarantees that for sufficiently small times the support of strong solutions locally does not increase. It turns out that this condition only depends on the diffusion growth exponent n in the equation above. Our approach combines a new version of Stampacchia's iteration lemma with weighted energy or entropy estimates. On account of numerical experiments, we conjecture that the aforementioned growth criterion is optimal.

Phase Segregation in Higher Dimensional Models

Dmitry Ioffe, Technion, Haifa

Winterbottom construction gives a phenomenological description of the equlibrated shape of a small particle placed on a solid substrate. Using recent results on the phase segregation in three and higher dimensions, the construction could be rigorously recovered in a scaling limit of the low temperature Ising type lattice models with finite range pair interactions. In this approach the influence of the substrate is modeled by a constant sign magnetic field which acts in a fixed number of microscopic bottom layers.

Incommensurate Phase Transitions

T. Janssen, University of Nijmegen, The Netherlands

In the last thirty years one has discovered many materials with sharp diffraction peaks but without lattice periodicity. These materials are called aperiodic crystals. One may distinguish several classes, such as modulated crystals incommensurate composites and quasicrystals. The Bragg spots are located on a vector Z-module of rank n $>$ 3. The symmetry of these aperiodic crystals can be described by an embedding in n dimensions. The 3D crystals then are intersections of an nD periodic structure and 3D physical space.

The additional dimensions are phase degrees of freedom. The origin of the incommensurate modulation is competition of ordering forces. The appearance can be explained with a discrete frustrated Φ^4 model. As function of the parameters at T=0, or as function of T in molecular field approximation or with Monte Carlo simulations an incommensurate phase is present in the phase diagram. Within the IC phase there is another phase transition at which the modulation function becomes discontinuous. Simultaneously a zero-frequency mode, different from an acoustic mode and corresponding to a shift in the additional dimensions, disappears and a phason gap opens up. With numerical calculations it has been shown that the zero-frequency mode also exists outside the validity range of the harmonic approximation. For low enough speeds there is a phase wave running through the crystal with very low friction. Similar phase transitions with the appearance of discontinuities, and analogous frictionless motion has been found in composites and quasicrystals.

Phase transitions in finite volumes

Roman Kotecký, Charles University, Praha

Phase transitions are revealed as nonanalyticities of thermodynamic potentials. To "see" their onset in finite volumes, one has to have a good understanding of asymptotic behaviour of corresponding infinite volume discontinuities. An alternative is to study asymptotic behaviour of the set of zeros of partition function on a torus.

A theory allowing to discuss such finite size effects is introduced on the simplest example of Ising model. It is shown how to reformulate it in terms of contour models, how to reinstate independence of contours in the case of nonvanishing external field and how to construct corresponding "metastable free energies" f_+ and f_- (the crucial notion of the Pirogov-Sinai theory).
Partition function on a finite torus T can be well approximated by the expression

$$Z_T \;\sim\; e^{-\beta f_+|T|} + e^{-\beta f_-|T|}$$

This is true also for complex values of external fields and allows for a detailed description of asymptotic loci of zeros.

Surface Relaxations on Crystal Growth

William T. Lee, University of Cambridge

Surface relaxations are distortions of the crystal structure in the vicinity of a surface. The physical origin of these relaxations lies in the fact that the environment of atoms near the surface is different from those in the bulk. Simple models suggest that this distortion decays exponentially as one moves away from the surface. Furthermore these simple models predict that if there are two opposite surfaces close to each other, then their respective relaxations will overlap and there will be an energy associated with this overlap. This energy takes the form of an attraction between the surfaces.

Standard theories of crystal morphologies assume that the surface energy is a constant and predict (e.g. by the Wulff construction) morphologies with the point group symmetry of the crystal system. An attractive interaction between surfaces, if it is sufficiently strong, has a destabilising effect on the growth morphology and stabilises a platelet morphology, even if such a morphology has a lower symmetry than that of the crystal system.

On the Convergence of Cluster Expansions

Salvador Miracle-Sole, Centre de Physique Théorique, Marseille

A simple proof of the convergence of cluster expansions for an abstract polymer system was presented.

Let $\mathcal{G}$ be a simple graph with a countable set $\mathcal{P}$ of vertices, also called polymers. If $\{\gamma, \gamma'\} \subset \mathcal{P}$ is an edge of the graph we say that two polymers are incompatible and write $\gamma \not\sim \gamma'$. Otherwise they are compatible and we write $\gamma \sim \gamma'$. A complex valued function $\phi(\gamma)$, $\gamma \in \mathcal{P}$, is given. For any finite subset $\Lambda \subset \mathcal{P}$, the partition function $Z(\Lambda)$ is defined by

$$Z(\Lambda) = \sum_{\substack{X \subset \Lambda \\ \text{compatible}}} \prod_{\gamma \in X} \varphi(\gamma)$$

The sum runs over all subsets X of Λ such that $\gamma \sim \gamma'$ for any two distinct elements of X. If X contains only one element, it is considered a compatible subset, and if $X = \emptyset$, the product is interpreted as the number 1.

A multi-index X on a set $\mathcal{P}$ is a function $X(\gamma)$, $\gamma \in \mathcal{P}$, taking non-negative integer values and such that $\operatorname{supp} X$ is a finite non-empty set. Then

$$\ln Z(\Lambda) = \sum_{X, \operatorname{supp} X \subset \Lambda} a^{\mathrm{T}}(X) \prod_{\gamma \in \mathcal{P}} \varphi(\gamma)^{X(\gamma)} = \sum_{X, \operatorname{supp} X \subset \Lambda} \phi^{\mathrm{T}}(X)$$

where the coefficients $a^{\mathrm{T}}(X)$ depend only on X (not on Λ), and $a^{\mathrm{T}}(X) \neq 0$ only if X is a cluster, i.e., only if the restriction of $\mathcal{G}$ to the vertices in $\operatorname{supp} X$ is a connected graph.

Theorem: Assume that there is a positive function $\mu(\gamma)$, $\gamma \in \mathcal{P}$, such that, for all $\gamma \in \mathcal{P}$,

$$|\varphi(\gamma)| \leq \left(e^{\mu(\gamma_0)} - 1\right) \exp\left(- \sum_{\gamma' \not\sim \gamma} \mu(\gamma') \right)$$

Then, for all $\gamma_1 \in \mathcal{P}$, we have

$$\begin{aligned} \sum_{X \in \mathrm{M}(\mathcal{P}),\, X(\gamma_1) \geq 1} |\phi^{\mathrm{T}}(X)| &\leq \mu(\gamma_1) \\ \sum_{X \in \mathrm{M}(\mathcal{P})} X(\gamma_1) |\phi^{\mathrm{T}}(X)| &\leq e^{\mu(\gamma_1)} - 1 \end{aligned}$$

The theorm is proved by an induction argument using the following relation: If $\gamma_0 \notin \Lambda$, then

$$Z(\Lambda \cup \{\gamma_0\}) = Z(\Lambda) + \varphi(\gamma_0) Z(\Lambda_0)$$

with $\Lambda_0 = \{\gamma \in \Lambda : \gamma \sim \gamma_0\}$, More details and references can be found in S. Miracle-Sole, Physica A 279, 244–249, 2000.

A cross–over for the scaling law of the first order correction to the LSW theory for domain coarsening

Barbara Niethammer, University of Bonn

(joint work with A. Hönig and F. Otto)

The classical theory by Lifshitz, Slyozov and Wagner describes diffusion limited coarsening of particles in the limit of vanishing volume fraction ϕ. We present a rigorous analysis in a stochastic setting which indentifies the scaling of the first order correctionto the LSW–theory. As a natural measure for the coarsening rate we take the rate of change of energy.

The relative deviation from the LSW–theory shows a cross–over between $\phi^{1/3}$ and $\phi^{1/2}$ when screening effects become important.

Large Deviations and Statistical Mechanics

Charles-Edouard Pfister (Department of Mathematics, EPF-Lausanne, Switzerland)

We expose the thermodynamical formalism via large deviations theory for a special class of systems, the classical spin systems with compact state space. The central point is to show how one can deduce equilibrium statistical mechanics from Boltzmann expression of the entropy. The thermodynamical properties of the system are expressed through a $\mathbb{R}^k$-valued macroscopic observable. Boltzmann entropy is equal to the rate function of a large deviations principle for this macroscopic variable (up to a constant and a sign). Statistical mechanics is recovered via the contraction principle and a large deviations principle for the empirical measure. By the contraction principle Boltzmann entropy is related to the Shannon (Kolmogorov-Sinai) entropy of translation invariant probability measures on the space of microscopic configurations. More precisely one has the following theorem. Let $x \in \mathbb{R}^k$ be the macroscopic state of the system, then the Boltzmann entropy $S(x)$ is equal to the supremum of the Shannon entropy $h_{Sh}(\mu)$ subject to the constraint that the expected value of the macroscopic observable in the state μ is x. One then proves that there exists at least one measure μ such that $S(x) = h_{Sh}(\mu)$, and each such measure is an equilibrium state, i.e. verifies the variational principle of statistical mechanics. For a large class of macroscopic observables this is equivalent to say that μ is a Gibbs measure, whose local specification can be computed from the macroscopic observable and the macroscopic state x.

On Stokes flow driven by degenerate surface tension

G. Prokert, Universität Leipzig

We consider a moving boundary problem for the "creeping" motion of a liquid drop governed by the Stokes equations and driven by surface tension. The surface tension coefficient is assumed to be variable and nonnegative, but not necessarily strictly positive. The problem can be reformulated as a fully nonlinear, nonlocal evolution equation for an $\mathbb{R}^N$-valued function on a fixed smooth reference manifold. In contrast to earlier work on this and related subjects, this approach avoids unnatural restrictions on the geometry of the problem.

The linearized evolution equation is degenerate parabolic. Its corresponding natural estimates, however, are in norms which are too weak for the treatment of the nonlinear problem. This "gap" can be bridged using a generalized chain rule describing the invariance of the problem under reparametrizations. Finally, well-posedness of the problem in a scale of Hilbert spaces can be shown by Galerkin approximations.

Similar techniques seem to be applicable to degenerate (quasistationary) phase change problems, e.g. of Hele-Shaw type.

Hypersurfaces with mean curvature given by an ambient Sobolev function

Reiner Schätzle (Departement der Mathematik, ETH Zürich)

We consider smooth, oriented $n-$hypersurfaces $\Sigma_j = \partial E_j$ with interior E_j whose mean curvature is given by the trace of a function in the ambient space $u_j \in W^{1,p}(\mathbb{R}^{n+1})$

$$\vec{\mathbf{H}}_{\Sigma_j} = u_j \, \nu_{E_j} \quad \text{on } \Sigma_j, \tag{1}$$

where ν_{E_j} denotes the inner normal of Σ_j . We investigate (1) when $\Sigma_j \to \Sigma$ weakly as varifolds and prove that Σ is an integral $n-$varifold with bounded first variation which still satisfies (1) for $u_j \to u$, $E_j \to E$. p has to satisfy

$$p > \frac{1}{2}(n+1)$$

and $p \geq \frac{4}{3}$ if $n = 1$. The difficulty is that in the limit several layers can meet at Σ which creates cancellations of the mean curvature.

Distortion Engineering — Modelling and Numerical Methods

Alfred Schmidt, Zentrum für Technomathematik, Universität Bremen

(joint work with M. Böhm and M. Wolff (Bremen), IWT Bremen, and E. Bänsch (Berlin))

"Distortion Engineering" is the name of the newly founded SFB 570 at Universität Bremen, located at the materials science department (IWT), with contributions from the Techno-Mathematics Center (ZeTeM). Subject of study are deformations during various production steps during the manufacturing of steel work pieces, both in experiments and simulations. We concentrate here on the late production step of surface hardening by quenching of a hot steel work piece.

We consider a model for isotropic thermo-elasticity with phase transitions, which is based on an austenite-pearlite-martensite phase transition model from D. Hömberg. Numerical simulations in two and three space dimensions are presented for the surface hardening of a steel rod and a gear wheel, performed with an adaptive finite element method, implemented in ALBERT.

Future projects are the enrichment of the (currently quite basic) model to include transformation induced plasticity (TRIP), more realistic phase transition models, and anisotropic elasto-plasticity, as well as mathematical and numerical analysis of the models.

Perseverance of the continous symmetry in 2D models: the case of singular interaction

S. Shlosman, CPT, Marseille

An old result of R. Dobrushin and the author tells that the continous symmetry of the interaction is not broken in the thermodynamic limit, provided the dimension is ≤ 2, and the interaction is finite-range and C^2. The common belief was that the C^2 condition is important and its absence might result in the phase transition.

In a recent paper, together with D. Ioffe and Y. Velenik we were able to show that it is not the case, and the continous symmetry is not broken, even for singular interactions.indent An old result of R. Dobrushin and the author tells that the continous symmetry of the interaction is not broken in the thermodynamic limit, provided the dimension is ≤ 2, and the interaction is finite-range and C^2. The common belief was that the C^2 condition is important and its absence might result in the phase transition.

In a recent paper, together with D. Ioffe and Y. Velenik we were able to show that it is not the case, and the continous symmetry is not broken, even for singular interactions.

Hysteresis operators in phase-field modelling

J. Sprekels, WIAS Berlin

Initial-boundary value problems for phase-field systems of the form

$$\mu(\theta)\, w_t \,+\, \mathcal{H}_1[w] \,+\theta\, \mathcal{H}_2[w] \;=\; 0 \tag{1}$$

$$(C_v\, \theta \,+\, \mathcal{F}_1[w]) \,-\, \kappa\, \Delta\theta \;=\; \psi(x,t,\theta) \tag{2}$$

for the unknown fields θ (absolute temperature) and $w = (w_1, \dots, w_M)$ (phase-field variables) are considered, where $\mathcal{H}_j = (\mathcal{H}_{j,1}, \dots, \mathcal{H}_{j,M}), j = 1, 2$, and $\mathcal{F}_1$ are hysteresis operators. Systems of the form (1), (2) with hysteresis operators naturally arise in the mathematical modelling of phase transitions, for instance, for the relaxed Stefan problem with double obstacle potential. In this connection, the phase-field variables $w_1, \dots, w_M$ denote generalized freezing indizes, i. e. they coincide with the negative time integral over the thermodynamic force driving the phase transition. Therefore, $w_1, \dots, w_M$ are the natural candidates for variables representing the accumulated thermodynamic memory of the system.

In this lecture, we focus on the special case when the operators $\mathcal{H}_1, \mathcal{H}_2$ are M-dimensional Prandtl-Ishlinskii operators. Such operators are widely used as realistic models for elasto-plastic strain-stress relations. Well-posedness and thermodynamic consistency can be shown for IBVPs for (1), (2), and asymptotic results for $t \to \infty$ are derived. The results are joint work with P. Krejčí (Prague).

Passage from atomistic to continuum models

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(joint work with G. Friesecke)

Continuum models like nonlinear elasticity theory illustrate the amazing flexibility of coarse–graining concepts. Although solids behave ultimately atomistic at very small scales, in the large body limit the concept proves to be surprisingly stable.

Scrutiny of the relation in a special case. We focus on the derivation of nonlinear elasticity theory via discrete models. In the case $d = 2$ we approximate the reference configuration $\Omega \subset \mathbb{R}^2$ of an elastic body by a sequence of lattices $\mathcal{L}^N \subset \Omega, N = 1, 2 \dots$. The interaction between two lattice sites $i, j \in \mathcal{L}^N$ is determined by pair potentials $V_{ij} : \mathbb{R}^2 \to \mathbb{R}$. The potential energy of a lattice deformation $q : \mathcal{L}^N \to \mathbb{R}^2$ is given by

$$E^N(q) = \frac{1}{|\mathcal{L}^N|} \sum_{(i,j)\in(\mathcal{L}^N)^2} V_{ij}(|q_i - q_j|).$$

Our objective is to find good bulk energy functions $W : \mathbb{R}^{2\times 2} \to \mathbb{R}$ so that for boundary values $g : \partial\Omega \to \mathbb{R}^2$

$$\lim_{N\to\infty} \min\{E^N(q) \mid q|_{\partial\mathcal{L}^N} = g\} = \inf\{\textstyle\int_\Omega W(D\varphi)\,\mathrm{d}x \mid \varphi|_{\partial\Omega} = g\}$$

holds. The Cauchy–Born assumption states that the discrete minimizers q^N approximate the continuum minimizer φ, cf. fig 1. Our approach to check the validity of the Cauchy–

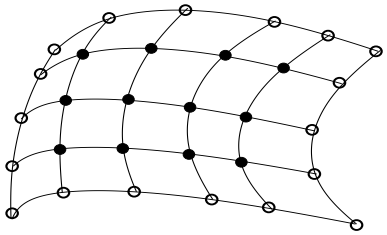

FIGURE 1. Illustration of the Cauchy–Born rule: The positions of the atoms approximate the continuum deformation

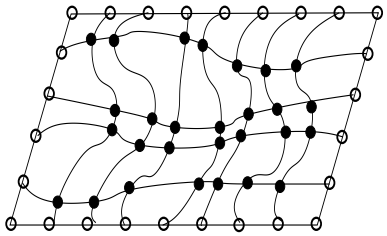

FIGURE 2. To compute the relaxed elastic energy we allow the atoms in the interior of the discrete domain "$\bullet$" to relax independently of the defomormation at the boundary. The restricted atoms are drawn with circles "$\circ$".

Born rule is to introduce the relaxed stored energy function

$$W^{\text{relax}}(F) =$$
$$\liminf_{N\to\infty} \min\{E^N(q) \mid \text{orientation preserving } q : \mathcal{L}^N \to \mathbb{R}^2,\ q|_{\partial\mathcal{L}^N} = i \mapsto F \cdot i\},$$

where we allow the atoms which are not part of the boundary to relax without restricting them kinematically, cf. fig 2. We are able to verify and falsify the validity of the Cauchy–Born rule in a simple case which involves only strictly convex interaction potentials. This demonstrates that the process of extracting continuum models from discrete models is quite delicate because the failure of the Cauchy–Born rule can not be detected on the level of a continuum model.

The example, which demonstrates the failure, relies heavily on the presence of the geometric nonlinearity which is caused by the invariance under ridgid body rotations i.e.

$$E^N(q) = E^N(Rq)$$

for all rigid body rotation $R \in SO(2)$.

Kinetic relations from "first principles"

L. TRUSKINOVSKY, UNIVERSITY OF MINNESOTA

We discussed a relation between

$$\ddot{u}_i = f'(u_{i+1} - u_i) - f'(u_i - u_{i-1}),$$

when $f(\cdot)$ is non-convex and its continuum analogy

$$u_{tt} = f''(u_x)u_{xx}.$$

To illustrate the difficulties associated with high frequency radiation accompanying propagation of subsonic phase boundary, we presented an exact solution in the form of travelling

wave of an associated toy model

$$\ddot{u}_i = u_{i+1} - 2u_i + u_{i-1} + f(u_i)$$

where $f(u_i)$ is double-well. We computed energy released by a moving defect and derived a semi-analytic kinetic relation. Evidence has been presented that the continuum closure of these discrete models must necessarily be thermodynamical.

Stability of Flat Interfaces During Semidiscrete Solidification

Andreas Veeser, Dipartimento di Matematica, Università degli Studi di Milano

The stability of planar interfaces with respect to a spatial semidiscretization of a solidification model is analyzed.

The considered model is the quasi-static approximation of the modified Stefan problem:

$$\begin{aligned} -\Delta\theta &= 0 \quad \text{in } \Omega^s(t) \text{ and } \Omega^l(t), \\ V + \left[\!\left[\frac{\partial\theta}{\partial n}\right]\!\right]_s^l &= 0 \quad \text{on } \Gamma(t), \\ \beta V + \gamma\kappa + \theta &= 0 \quad \text{on } \Gamma(t), \end{aligned}$$

where θ denotes the (scaled) temperature, $\Omega^s(t)$ the solid part, $\Omega^l(t)$ the liquid part, $\Gamma(t)$ the separating interface, n its normal (pointing into the liquid), V its normal velocity, κ its curvature (positive, if the solid is convex), $[\![\cdot]\!]_s^l$ the jump across the interface, β the kinetic coefficient, and γ the solid-liquid surface tension.

The spatial semidiscretization bases on finite elements. More precisely, the interface is represented as the graph of a continuous finite element function and moving (or: time-dependent isoparametric) finite elements are used for the temperature.

The stability analysis bases on an argument developed by Mullins and Sekerka for the undiscretized case. The main result shows that the semi-discrete problem exhibits a stability regime that mimics the continuous one only if the discretization is fine enough.

Kinetic and Stochastic Effects in the Dynamics of Coarsening

Juan J. L. Velázquez, Madrid

The classical Lifshitz-Slyozov-Wagner (LSW) model of coarsening is given by the following system of equations:

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial R}\left(\left(-\frac{1}{R^2} + \frac{1}{\langle R\rangle}\right) f\right) = 0 \tag{1}$$

$$\langle R\rangle = \frac{\int_0^\infty R f\,(R,t)\,dR}{\int_0^\infty f\,(R,t)\,dR} \tag{2}$$

The function $f = f\,(R,t)$ describes the distribution in the space of radii of the sizes of a set of particles whose evolution is driven by diffusion and interfacial energy. More precisely, system (1), (2) is a "mean field theory" that is derived assuming that a set of spherical particles filling a small volume fraction of the space and in whose boundaries the classical Gibbs-Thomson equation is satisfied, evolves according to the usual Stefan law (cf. [LS]).

The classical theory of coarsening states that the average radius of the system of particles described by (1), (2) grows according to the power law $(t)^{1/3}$. This conclusion is reached

using the fact that system (1), (2) admits a family of self-similar solutions, and some stability considerations presented in [LS] suggest that one particular solution in the class of self-similar solutions should be preferred.

It has been recently shown , however, that the asymptotic behaviour of the solutions of (1), (2) is extremely sensitive on the initial distribution of radii, and more precisely, on the asymptotic behaviour of the initial distribution of radii near the maximum radius (cf. [NP]). In particular for suitable distributions of initial radii solutions can behave for long times as the "supposedly wrong" self-similar solutions, of even in a non-self-similar manner.

It is possible to consider several regularizations of the model (1), (2) that could perhaps overcome this problem. The system (1), (2) can be formally considered as the limit for large particles of the classical Becker-Döring system of equations:

$$\frac{\partial c_\ell}{\partial t} = J_{\ell-1} - J_\ell \tag{3}$$

$$J_\ell = a_\ell c_\ell c_1 - b_{\ell+1} c_{\ell+1} \tag{4}$$

$$\sum_{\ell=1}^{\infty} \ell c_\ell = \rho \tag{5}$$

Approximating (3)-(5) by a second order partial differential equation can be seen that only the self-similar solution suggested in [LS] provides a possible long time asymptotics for (3)-(5), at least in the class of self-similar behaviours. Precise description of the asymptotics of the solutions as $t \to \infty$ can also be obtained (cf. [V1]).

Another possible regularization of the system (1), (2) is to introduce corrections to the mean field theory, and to estimate the effect of such a corrections in the dynamics of the solutions. Assuming that the particles are initially distributed in a stochastically homogeneous manner it is possible to compute the leading corrective terms to (2), (2) in the limit of very small volume fractions (but not zero), and to check that the effect of such corrections is too small to modify the dynamics of (1), (2) in a meaningful manner. More precisely, the solutions that are initially close to some of the "wrong" self-similar solutions remain close to such solutions for long times and they do not approach to the solution suggested in [LS] for those times in which a continuous (non stochastic) description of the particles is possible (cf. [V2]).

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Unique global solvability for initial-boundary value problems in one-dimensional thermoviscoelasticity

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The balance laws for mass, momentum and energy are considered for a broad class of one dimensional thermoviscoelastic materials. We prove the unique global solvability for the one-dimensional initial-boundary value problem corresponding to *pinned* endpoints held at

constant temperature [1]. The key step in the proof hinges on a new estimate for the density, via a previously unsuspected generalisation of the celebrated approach of Kazhikhov and Shellukhin [2]. Their result applied to a viscous, heat-conducting ideal gas; i.e., the compressible Navier-Stokes. Our approach also applies to all boundary conditions involving pinned or stress-free endpoints which are either held at constant temperature or insulated. An additional and novel feature of the theory is that *solid-like* and *gaseous* materials are treated in a unified way. However, this does not yet complete our understanding of the global solvability issue, since our methods do not apply to temperature dependent viscosity.

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Local minimizers in micromagnetics

Matthias Winter, Universität Stuttgart

(joint work with A. Taheri and J.M. Ball)

Let $\Omega \subset \mathbf{R}^3$ be a smooth bounded domain and consider the energy functional

$$J_\varepsilon(m) := \int_\Omega \left(\frac{1}{2\varepsilon}|Dm|^2 + \psi(m) + \frac{1}{2}|h-m|^2 \right) dx + \frac{1}{2}\int_{\mathbf{R}^3} |h_m|^2 \, dx.$$

Here ε is a small non negative parameter and the space of admissible functions for m is the Sobolev space of vector-valued functions $W^{1,2}(\Omega;\mathbf{R}^3)$ which satisfy the pointwise constraint $|m(x)|^2 - 1 = 0$ for a.e. $x \in \Omega$. The integrand $\psi : \mathbf{S}^2 \to \mathbf{R}$ is assumed to be a sufficiently smooth non negative density function with a multi-well structure. The function $h_m \in L^2(\mathbf{R}^3;\mathbf{R}^3)$ is related to m via Maxwells equations. Finally $h \in \mathbf{R}^3$ is a constant vector. The energy functional J_ε arises from the study of continuum models for ferromagnetic materials known as *micromagnetics* developed by W. Brown (1963).

In this talk we aim to construct local energy minimizers for this functional. Our approach is based on studying the corresponding Euler-Lagrange equation and proving a *local existence* result for solutions close to a fixed constant solution. Our main device for doing this is a suitable version of the implicit function theorem. We then show that these solutions are *local minimizers* of J_ε in appropriate topologies by using certain sufficiency theorems for local minimizers.

Our analysis is applicable to a much broader class of functionals than the ones introduced above and on the way of proving our main results we reflect on some related problems.

Polyconvex Frame-Indifferent Functions in Two Space Dimensions

Johannes Zimmer, Technische Universität München

We are interested in polyconvex functions which satisfy the axiom of frame indifference. The aim is to extend Ball's famous theorem on isotropic polyconvex functions (ARMA 77) to frame-indifferent functions. We get a similar condition to describe a large class of frame-indifferent polyconvex functions which include all possible symmetries. The crucial point in this construction is the use of algebraic methods and invariant theory. We will briefly indicate extensions to the three-dimensional case.

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