

MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

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Mathematische Behandlung von Phasenübergängen

10.05. - 16.05.1998

The meeting has been organized by Hans-Wilhelm Alt (Bonn), Stephan Luckhaus (Leipzig) and Mete Soner (Princeton). A main focus of the conference was the relationship between microscopic and macroscopic models for phase transitions. Some of the subjects treated in the talks are:

- phase transitions in systems with long range interactions,
- models from microscopic statistical mechanics (Ising models, Kac-Ising models, ...),
- relationship between microscopic, mesoscopic and macroscopic models,
- Stefan problems with Gibbs-Thomson Law,
- nucleation phenomena,
- mean curvature flow,
- surface diffusion,
- microstructures in martensitic phase transformations,
- Ginzburg Landau models,
- superconductivity,
- phase transitions in multi-phase systems.

## ABSTRACTS

GIOVANNI ALBERTI:

### A young measure approach to two-scale problems

When considering certain variational problems  $\mathcal{P}_\epsilon$  which arise for instance in the modelization of microstructures in martensitic interfaces (with  $\epsilon$  a small dimensionless parameter), the analysis of the asymptotic behaviour of the solutions  $u_\epsilon$  as  $\epsilon$  tends to zero may require different mathematical tools. In this talk I briefly summarize a Young measure approach introduced in a joint work with S. Müller to describe the asymptotic behaviour of the minimizers of the one-dimensional functionals  $I_\epsilon(u) := \int \epsilon^2 \ddot{u}^2 + (\dot{u}^2 - 1)^2 + au^2$ .

LUIGIO AMBROSIO:

### A measure theoretic approach to mean curvature flow in higher codimension

The convergence as  $\epsilon \downarrow 0$  of solutions  $u^\epsilon$  of the Ginzburg-Landau system

$$u^\epsilon_t = \Delta u^\epsilon + \frac{1}{\epsilon^2} u^\epsilon (1 - |u^\epsilon|^2) \quad u : \mathbf{R}^n \rightarrow B_1 \subset \mathbf{R}^2$$

can be used, with suitable initial conditions, to approximate the  $(n - 2)$ -dimensional mean curvature flow. Convergence results before the appearance of singularities have been proved by Rubinstein-Pismen, Jerrard-Soner and Lin. In a joint work with H. M. Soner (which will be published in the Annali of the Scuola Normale Superiore) we have proved convergence to a Brakke flow for all positive times. The proof is based on a generalization of the classical theory of varifolds and on a detailed analysis of the gradient Young measures arising in the limit. Partial results in codimension  $k > 2$  have also been obtained.

(joint work with Halil Mete Soner)

PATRICIA BAUMAN:

### A three dimensional superconductor in a strong magnetic field

From a mathematically rigorous analysis of the Ginzburg-Landau model, we investigate the behaviour of a three-dimensional superconducting material in a uniform magnetic field of strength  $h$ . We show that the material exhibits vortex filaments of normal (nonsuperconducting) material when it is a type II superconductor and  $h$  is sufficiently large but below the upper critical value. We also describe the nature of the induced magnetic field and order parameter in a three dimensional ball of superconducting material, which is quite different from the two dimensional case of a cylinder with fixed cross section.

GIOVANNI BELLETTINI:

Allen-Cahn type approximation to crystalline motion by mean curvature

Assume that  $\varphi : \mathbb{R}^N \rightarrow \mathbb{R}^+$  is a given norm on  $\mathbb{R}^N$ , and let  $\varphi^0 : \mathbb{R}^N \rightarrow \mathbb{R}^+$  be the dual of  $\varphi$ . We are interested to the case in which the two convex sets  $\{\varphi^0 \leq 1\}$ ,  $\{\varphi \leq 1\}$  are non smooth and have flat portions. Let  $T^0 = \frac{1}{2}\partial(\varphi^0)^2$  be the duality mapping, where  $\partial$  denotes the subdifferential. Let  $\epsilon > 0$  and consider the problem

$$\begin{cases} u_t = \nabla \cdot \xi - \frac{1}{\epsilon^2} \varphi(u) + \frac{c_0}{2\epsilon} g, \\ \xi \in T^0(\nabla u), \\ u(0, \cdot) = u_0, \end{cases}$$

coupled with suitable boundary conditions, where  $\psi$  is the derivative of a double well potential,  $c_0$  is a constant, and  $g = g(x, t)$  ist given. Considering the asymptotic behaviour of the solutions of (1) we can prove a comparison principle between  $\phi$ -regular flows in  $N$  dimensions and for  $g = g(t)$ . This result includes the comparison principle in the crystalline case. We next discuss the convergence of the solutions to (1) to  $\phi$  regular flows as  $\epsilon \rightarrow 0$ . The convergence result is optimal for  $N = 2$ ,  $\phi$  crystalline,  $g = g(t)$  or  $g = g(x, t)$  "small", in the sense that no new facets create. We finally focus the attention to the case  $N = 3$ ,  $\phi$  crystalline,  $g = 0$  and show by some examples that, during motion by crystalline mean curvature, creation of new facets is more the rule than the exception.

(work in collaboration with M. Novaga and M. Paolini)

ANTON BOVIER:

Phase transitions in spin systems with long range interactions

In 1963, Marc Kac proposed a class of models that allowed to recover the van der Waals theory including the Maxwell construction as an asymptotic result from microscopic statistical mechanics. This was obtained by choosing an interaction of the form  $J_\gamma(x - y) \equiv \gamma^d J(\gamma(x - y))$  where  $J$  is some function of bounded support or rapid decay and  $\gamma$  a scaling parameter allowing to send the range of the interaction to infinity. In recent years, there has been renewed interest in such models since they also permit to derive local field theories (of Ginzburg-Landau type) and to study the connection of such theories to lattice theories in a rigorous way. An important question here is to understand to what extend the properties of the  $\gamma \downarrow 0$  limit reflect properly those of the system at small but finite  $\gamma$ . In particular, I discuss the issue of the continuity of the critical temperature as a function of  $\gamma$  at 0. This property, which obviously fails in one space dimension, has been established only recently in the context of the Ising-Kac model in dimension  $d \geq 2$  [CP,BZ].

In my view these question will be of particular interest in the context of spin systems with quenched disorder. For such models it is far from obvious to derive ad hoc appropriate continuum field theories, and the study of Kac versions of such models may be helpful in

order to understand what is going on here. So far, a few examples have been considered: the dilute Kac-Ising model [BO], the Kac-Ising model with random magnetic field [COPi], and the Kac-Hopfield model [BGP]. So far, results concern the Lebowitz-Penrose theorems, and the distribution of typical overlap profiles in the one dimensional case.

[Bo] Th. Bodineau: *Interface for one-dimensional random Kac potentials*,  
Ann. Inst. Henri Poincaré **33**, 559-590 (1997).

[BGP] A. Bovier, Gayrard and P. Picco: *Distribution of overlap profiles in the one-dimensional Kac-Hopfield model*,

[BZ] A. Bovier, M. Zahradník: *The low temperature phase of Kac-Ising models*, J. Stat. Phys. **87**, 311-332 (1997) Commun. Math. Phys. **186**, 323-379 (1997).

[CP] M. Cassandro, E. Presutti, *Phase transitions in Ising systems with long but finite range interactions*, Markov Proc. Rel. Fields **2**, 241-262 (1996).

[COPi] M. Cassandro, E. Olivieri, P. Picco, *Typical configurations for one dimensional random field Kac model*, preprint available at mp-arc (98-35)(1998)

GERO FRIESECKE:

Thermodynamics from first principles

The relationship between the atomistic (i. e. quantum mechanical) and the continuum description of solids is still poorly understood. While workers in physics and materials science are nowadays succeeding in predicting macroscopic data such as elastic constants via 'ab initio' numerical codes, little rigorous work is available, with the exception of an important paper by C.Fefferman (1985).

The mathematical challenges posed by a direct passage from quantum to continuum mechanics are deep and numerous. We will describe recent progress (joint with R. D. James, University of Minnesota, Minneapolis) and explain in particular why the common approximation of atoms simplified into classical point particles is inadequate for solids. One of its spectacular failures is its misprediction of the number of elastic constants ('Cauchy relations') even when all interactions between all particles are retained and the exact interatomic pair potential delivered by quantum mechanics is used. This illustrates that unlike in the kinetic theory of gases, in solids a dominant role is played by quantum, many-body correlations.

HARALD GARCKE:

Triple point evolution in Cahn–Hilliard systems with degenerate mobility

Isotermal phase separation in multicomponent systems can be modeled by a system of Cahn–Hilliard equations. In such a system the diffusional mobility matrix in general can be expected to be dependent on the concentration of the components. In regions in which one component is predominant, the mobility tends to be much smaller than in regions in which there is a mixture of different components. This implies that diffusion in interfacial regions is relatively enhanced. In particular, this phenomenon becomes more pronounced at low temperatures where entropy contributions are smaller. Therefore, it is reasonable to consider systems of Cahn–Hilliard equations in which the mobility matrix depends on the concentrations of the different components. In particular the mobility matrix in general degenerates in the pure components.

In my talk I will study a singular limit for a system of Cahn–Hilliard equations with a degenerate mobility matrix near the deep quench limit. Via formal asymptotics, this singular limit is seen to give rise to geometric motion in which the interfaces between the various pure phases move by motion by minus the surface Laplacian of mean curvature. These interfaces may couple at triple junctions whose evolution is prescribed by Young’s law, balance of fluxes, and continuity of the chemical potentials. Short time existence and uniqueness is proven for this limiting geometric motion in the parabolic Hölder space  $C_{t,p}^{1+\frac{\alpha}{2}, 4+\alpha}$ ,  $0 < \alpha < 1$ , via parametrization of the interfaces.

(joint work with Amy Novick–Cohen)

In a second part a finite element method to approximate solutions of the degenerate Cahn–Hilliard equation is introduced. The numerical method is stable in space dimensions 1, 2, 3 and convergence will be shown in one space dimension. Finally, I illustrate the difference in the qualitative behaviour between solutions of the Cahn–Hilliard equation with constant and with degenerate mobility by some numerical examples.

(joint work with John Barrett and James Blowey)

DIETMAR HÖMBERG:

A continuum mechanical approach to the derivatiuon of interface conditions

Starting point for our investigations is the problem of pressure resistance welding, where electric potential, stress tensor, velocity field and temperature have to be calculated.

To this end we discuss the respective interface conditions on the free surface between solid and liquid.

Beginning with a general balance law, we derive jump conditions for mass, momentum and energy, recovering the classical laws in special cases. We conclude with some remarks on Gibbs-Thomson laws.

(joint work with W. Dreyer, Berlin)

**DIMA IOFFE:**

Droplet concentration in effective interface models with convex potentials

Rigorous justification of equilibrium crystal shapes (Wulff construction) directly from a picture of microscopic interactions is a pending problem of mathematical statistical mechanics, which has been solved so far only for a limited class of two-dimensional models, e.g. nearest neighbour Ising model. An essential step on the way to higher dimensions is to develop a coarse graining calculus of microscopic phase boundaries. Such a calculus has been proposed in the context of the simplified effective interface model of the following type:

Let  $D \subset \mathbb{R}^d$  be sufficiently nice, and define its discretization  $D_N$  as  $D_N = D \cap \frac{1}{N}\mathbb{Z}^d$ . The effective interface  $\xi_N(x)$  over  $D$  is an interpolation of the scaled random surface  $\{h_i\}$  over  $D_N$  subject to the Hamiltonian

$$H_N(h) = \sum_{\langle ki \rangle} V(h_k - h_i),$$

where the summation is over nearest neighbours of  $\frac{1}{N}\mathbb{Z}^d$ , and the heights  $h$  are assumed to be pinned outside  $D_N$ , that is  $k \notin D_N \Rightarrow h_k = 0$ . Then, for every symmetric potential  $V$  satisfying

$$\frac{1}{c} \leq V'' \leq c,$$

the fluctuations of  $\xi_N$  are governed on the exponential scale by the functional

$$u \mapsto \int_D \sigma_V(\nabla u) dx,$$

where  $\sigma_V$  is the surface tension of the model.

**ROBERT JERRARD:**

Functions of bounded higher variation

We define the class of functions of bounded  $n$ -dimensional variation (BnV). These are functions  $u : \mathbb{R}^m \rightarrow \mathbb{R}^a \wedge (m \geq n)$  for which the distributional determinants of every  $n \times n$  submatrix of  $\nabla u$  is a signed Radon measure. Such functions "naturally" support singular

sets of codimension  $n$ . As such they can be useful in describing phenomena like vortex filaments which involve structures of codimension  $n \geq 2$ .

We prove that a version of Federer's coarea formula holds in this general context. We also show that, for  $u \in \text{BnV}(\mathbb{R}^m; \mathbb{R}^n)$  such that  $|u| = 1$  a. e., the Jacobian measure is an integer multiplicity measure supported on an  $m - n$  dimensional rectifiable set.

(joint work with G. Alberti and M. Soner)

MARKOS KATSOULAKIS:

Multiscale analysis for phase transition problems

In the first part of the talk we discuss the derivation of macroscopic interface evolution equations from Ising models with Kač potentials and general spin flip dynamics (joint work with P. E. Souganidis). We obtain an anisotropic, curvature-dependent, local law for the motion of interfaces and identify the mobility and surface tension from the microscopic variables (interaction potential, microscopic dynamics) of the Ising System.

Finally, we discuss applications and extensions of the aforementioned techniques to Chemical Vapor Deposition (CVD) processes (joint work with D. Vlachos). We obtain from the surface microprocesses (adsorption, desorption, reaction, surface diffusion), mesoscopic and macroscopic PDEs, and couple them in suitable scales to the continuum models of the gas phase.

MICHAEL KIESSLING:

Phase transitions in systems with long range forces

This talk is about systems of particles with pair interaction that have such a weak decay at large distances that the traditional thermodynamic limit (bulk limit) does not exist. Prominent examples of such systems are: classical hard balls with gravitational interactions; point particles with Coulomb interactions and 1 sign of charge; point vortices in an Euler flow, having logarithmic interactions and 1 sign of vorticity; Fermions with gravitational interactions. The problem is to construct a counterpart of the T-limit, where  $N \rightarrow \infty$ , such that  $\frac{1}{N}S \rightarrow$  limit, where  $S$  is the entropy. Using the example of point vortices, it is explained that such a limit exists on the energy scale  $E = N^2\epsilon$ ,  $\epsilon$  fixed, thus  $\frac{1}{N}S(N^2\epsilon) \rightarrow s(\epsilon)$  the entropy  $s(\epsilon)$  satisfies a variational principle that leads to a nonlinear PDE with multiple solutions and, thus, phase transitions.

HERBERT KOCH:

Large time regularity of solutions to the porous medium equation

We consider the porous medium equation

$$\rho_t = \Delta \rho^m$$

with  $m > 1$ . It is well known that solutions which have compact support initially are compactly supported for all times. We prove that locally nondegenerate solutions have a smooth pressure up to the boundary of the support. Moreover the boundary of the support is smooth for those solutions. All solutions under some weak restrictions on the initial data are nondegenerate for large times and hence smooth. The proof relies on modified Gaussian estimates for the fundamental solution of a linear degenerate parabolic (subelliptic) equation with measurable coefficients.

WILHELM MERZ:

Dopant diffusion in homogenous structures  
(modelling, analysis and numerical simulation)

We consider a general model for phosphorus diffusion in silicon (homogeneous material) under extrinsic doping conditions. At such high concentrations we have to include the charged species and the internal electric field of the crystal, both of which can have profound effects on diffusion. In principle, this leads to a very large number of drift-diffusion-reaction equations: one for each charge state of every species, plus one Poisson equation to describe the internal electric field (in terms of the electron/hole concentration). The number of equations can be reduced substantially by making additional assumptions on the distribution of charge states and local equilibrium assumptions concerning the reaction terms. We consider model

$$\begin{aligned} \frac{\partial C_\alpha}{\partial t} - \operatorname{div} \left\{ \mathcal{D}_\alpha(\psi) [\nabla C_\alpha + Q_\alpha(\psi) C_\alpha \nabla \psi] \right\} &= R_\alpha(\mathbf{C}, \psi), \\ -\frac{\epsilon}{e} \Delta \psi + 2n_i \sinh(\psi) &= \sum_\alpha Q_\alpha(\psi) C_\alpha, \end{aligned}$$

with appropriate initial- and boundary conditions. The index  $\alpha = 1, \dots, N$ , denotes the different species, whereas  $\mathcal{D}_\alpha(\psi)$  and  $Q_\alpha(\psi)$  are the diffusivities and the averaged charges, respectively. The reaction rates  $R_\alpha(\mathbf{C}, \psi)$  depend on all concentrations and the electrostatic potential as well.

We formulate an energy functional for our system of equations and deduce from it a series of energy estimates which form a good basis for further a-priori estimates required for the fixed point argument to prove the existence of strong solutions.



The resulting model turns out to be very interesting for numerical investigation. We solve the problem numerically in two space dimensions with the adaptive finite element program KARDOS (J. Lang, ZIB) and present numerical simulations concerning the drift-diffusion-reaction problem.

H. MÜLLER-KRUMBHAAR:  
The growth of a nucleus

First order phase transitions evolve through the formation and growth of a supercritical nucleus. A theory for the morphology-diagram of possible structures in diffusional growth is presented [1]. The results were obtained by various numerical and analytical methods. The main physical control parameters are undercooling  $\Delta$ , anisotropy of surface tension  $\epsilon$  and the strength of noise. Basic patterns are dendrites and seaweed. The building block of the dendritic structure in two dimensions is a doublon [2]. The transition between these structures shows a jump in the growth velocity. We also describe the structures and velocities of fractal dendrites and doublons resulting from the action of noise. The possible competition [3] between different growing substructures within a growth-front is shortly discussed. Finally recent results on the three-dimensional growth [4] of a supercritical nucleus are presented.

- [1] E. Brener, H. Müller-Krumbhaar and D. Temkin, Phys. Rev. E **54** (1996) 2714
- [2] T. Ihle and H. Müller-Krumbhaar, Phys. Rev. Letters **70**, 3083 (1993) Phys. Rev. E **49**, 2972 (1994)
- [3] H. Müller-Krumbhaar, M. Zimmer, T. Ihle, Y. Saito, Physica A. **224**, 322 (1996)
- [4] Th. Abel, E. Brener and H. Müller-Krumbhaar, Phys. Rev. E **55**, 7789 (1997)

BRITTA NESTLER:  
A multiphase-field model and its application to numerical simulations of moving phase boundaries and junctions

We introduced the formulation of a general class of diffuse multi-phase order parameter (or phase-field) models which include surface energy and time relaxation anisotropy.

In the original work (H. Garcke, B. Nestler, B. Stoth, Physica D, **115** (1998), 87-108), formally matched asymptotic expansions were used to determine the asymptotic limit when a small parameter related to the thickness of the interface tends to zero. We stated the results that we obtained in the case of anisotropic Allen-Cahn systems. At interfaces the anisotropic form of the Gibbs-Thomson equation is recovered, whereas at triple junctions a force balance can be derived which is known as Young's law and which in the anisotropic

case includes shear forces (Herring torque terms) acting normal to the interface.

Next, we gave explicit expressions for the free energies. In a series of simulations we have tested the different choices of bulk free energies that we proposed in order to find the best calibration between numerical and physical parameters. Since, in these experiments, a higher order variant of an obstacle potential has proved to have the best properties, we chose this potential for our simulations.

Finally, we presented numerical simulations of isotropic, anisotropic and crystalline phase systems which support the formal asymptotic analysis relating a multi order parameter Allen–Cahn system to a multi phase interface problem with curvature dependent evolution of the interfaces and angle conditions at triple junctions.

We compared our numerical computations of phase boundaries and triplejunctions with exact solutions. In addition, we numerically studied the symmetry condition of two adjacent triple junctions, we calculated the stability of quadruple junctions in a four phase system and finally, we showed a simulation of grain growth starting from many grains initially.

(joint work with Harald Garcke and Barbara Stoth)

BARBARA NIETHAMMER:

Self-similarity and instability in the LSW-theory of Ostwald ripening

The classical LSW-theory of coarsening predicts asymptotically self-similar behavior for the size distribution of a dilute system of particles that evolve by diffusional mass transfer with a common mean field. We consider the long-time behavior of measure-valued solutions for systems in which particle size is uniformly bounded, i.e., for initial measures of compact support.

We establish that the long-time behavior of the size distribution depends sensitively on the initial distribution of the largest particles in the system. Convergence to the classically predicted smooth similarity solution is impossible if the initial distribution function is comparable to any finite power of distance to the end of the support. We also give a necessary criterion for convergence to other self-similar solutions, and conditional stability theorems for some such solutions.

(joint work with R. L. Pego)

JOHN OCKENDON:

Mush and dislocations

The talk began with a description of the modelling of a solid superheated by volumetric heating. The history of this problem was traced back to a work in 1958 when Oleinik and Kamenomostskaya proposed a weak formulation of the relevant Stefan problem. Then came the realisation that it could predict a mushy region (Atthey 1973) and more recently there have been speculations about a microscopic nucleation model (Lacey/Taylor 1983) and the possible applicability of the phase field model (Fife & Gill 1989, 91 and Radkevich et al 1998).

Most of the talk concerned the modelling of dislocation dynamics in an elastic crystal. Classical Volterra theory describes a prescribed dislocation as a line singularity in the curl of a suitable elastic potential. Currently, it is then necessary to use an ad-hoc theory of slip planes and mobility laws to predict the dynamics. Unlike the case of vortices and superfluids, when a continuum core model can be used to predict the dynamics via matched asymptotic expansions, a discrete core is inevitable for a dislocation. Simple paradigms for such a core were proposed as candidates for models which could have a far field continuum limit. However, these models might light the sensitive dependence on the parameters in the core model and, in particular, the difficulty of determining the small Peierls stress that is needed to move the dislocation.

ENZA ORLANDI:

Results for a non-local equation with a conservation law,  
in a phase transition regime

I consider a non-local evolution equation that describes the evolution of the local magnetization in a continuum limit of an Ising spin system with Kawasaki dynamics and Kac potentials.

I study the evolution at subcritical temperatures for which there are two local equilibria, and prove a local nonlinear stability result for the minimum free energy profile for the magnetization at the interfaces between regions of these two different local equilibrium. These minimum free energy profiles are denoted fronts. The rate of relaxation to the front is given, obtaining power-law bounds.

Moreover, rescaling time and space in a suitable way, it is possible to prove that level surfaces of pollutions of this non-local evolution equation tend to solutions of Hele-Shaw problem under the assumption that classical solution of the latter exists.

The results given are based on the following papers.

[1] J. L. Lebowitz, E. Orlandi, E. Presutti: *A particle model for spinodal decomposition*, J. Stat. Phys. 63, 933-974 (1991)

[2] G. Giacomin, J. Lebowitz: *Phase segregation dynamics in particle systems*

with long range interactions I: Macroscopic limits, J. Stat. Phys. 87, 37-61 (1997)

- [3] G. Giacomini, J. Lebowitz: *Phase segregation dynamics in particle systems with long range interactions II: Interface motions*
- [4] E. A. Carlen, M. C. Carvalho, E. Orlandi: *Stability of fronts for a non-local phase Kinetics equation with a conservation law*, Preprint 1998
- [5] E. A. Carlen, M. C. Carvalho, E. Orlandi: *Convergence to Hele-Shaw problem for phase Kinetics equation with a conservation law*, (in preparation)

FERNANDO REITICH:

Calculation of the overall magnetic properties of magnetorheological fluids

Magnetorheological (MR) fluids constitute an example of controllable ("smart") fluids whose rheological properties vary in response to an applied magnetic field. These fluids typically consist of micron-sized magnetizable particles, dispersed in a non-magnetic fluid.

The essential characteristic of MR fluids is that they may be continuously and reversibly varied from a state of free flowing liquids in the absence of a magnetic field to that of stiff semi-solids under a moderate field.

In this talk we will present some preliminary results on the calculation of the overall magnetic response of MR fluids. We will show that simple periodic effective medium approximations deliver results that are in good agreement with experimental data at low field intensities, provided these measurements are taken after a period of time that allows for the structural arrangement of particles. To model this transient regime, on the other hand, we will present a model for the simulation of the particle dynamics. This model, in its present state, takes into account the full magnetic particle-particle interaction (computed via a Fast Multipole Algorithm) as is therefore well-suited for the calculation of the magnetic signature of the fluid.

TRISTAN RIVIÈRE:

A uniqueness result for the minimizers of the Ginzburg-Landau functional in dimension 2

We consider the minimizers of the non-gauge invariant Ginzburg-Landau functional

$$E(u) = \int_{\Omega} |\nabla u|^2 + \frac{\lambda}{2} (1 - |u|^2)^2$$

where  $u : \Omega \rightarrow \mathbb{C}$ , for large coupling parameters  $\lambda = 1/\epsilon^2$ , on a bounded 2-dimensional

simply connected domain  $\Omega$  and for a given boundary condition  $u = g : \partial\Omega \rightarrow S^1$  whose degree  $d$  is positive. As  $\epsilon$  tends to zero, it has been proved by F. Bethuel, H. Brezis and F. Hélein that, from any sequence of minimizers of  $E$ , we can extract a subsequence which converges to the limit

$$u_* = \prod_{j=1}^d \frac{z - a_j}{|z - a_j|} \exp(i\phi)$$

where  $\Delta\phi = 0$  in  $\Omega$  and  $u_* = g$  on  $\partial\Omega$ . Moreover they proved that the location of the  $a_j$ 's is given by the following problem :  $(a_j)$  has to minimize a function  $W : \Omega^d \rightarrow \mathbb{R}$  which only depends on  $\Omega$  and  $g$ . With F. Pacard we proved that, if two sequences  $u_n = u_{\epsilon_n}$  and  $v_n = v_{\epsilon_n}$  of minimizers of  $E$  converge to the same  $u_*$  as  $\epsilon_n$  tend to zero, such that the corresponding  $(a_j)$  is a non-degenerate minimizer of  $W$ , then, for  $n$  large enough, one has

$$u_n = v_n$$

JACOB RUBINSTEIN:

Phase transition curves in mesoscopic superconductors

We analyse the phase transition curve  $T_c(\Phi)$  for mesoscopic superconductors. Particular attention is given to the multiply connected domains, where Little Parks oscillations are pronounced. It is shown that the phase transition diagram and properties are very sensitive to variations in the geometry. We also describe some recent work of Sternberg and his coworkers on the  $T_c(\Phi)$  curve in mesoscopic simply connected domains.

(joint work with Jorge Berger and Michelle Schatzman)

PIOTR RYBKA:

The crystalline version of the planar modified Stefan problem with kinetic undercooling and its properties

The author studies the modified Stefan problem in the plane for polygonal interfacial curves. Existence and uniqueness of local in time solutions is shown. Geometric properties of the flow are studied if the Wulff shape is a regular  $N$ -sided polygon and the initial interface has sufficiently small perimeter. Namely, if the isoperimetric quotient of the initial interface differs from the isoperimetric quotient of the Wulff shape by no more than  $4\pi/N^3$ , then the interface shrinks to a point in finite time and the isoperimetric quotient decreases.

REINER SCHÄTZLE:

Global existence for a nonlocal mean curvature flow as a limit of a parabolic-elliptic transition model

We consider the mean curvature flow in its level set formulation coupled with an elliptic equation

$$\begin{aligned} \partial_t \psi - |\nabla \psi| \nabla \left( \frac{\nabla \psi}{|\nabla \psi|} \right) + cv |\nabla \psi| &= 0, \\ -\Delta v + v &= 2\chi_{\{\psi > 0\}} - 1, \end{aligned} \quad (1)$$

where  $\chi$  denotes the characteristic function.

In [3], [5] and [7], mean-curvature flow coupled with a parabolic equation or an elliptic equation whose right-hand side depends continuously on  $\psi$  was studied. Then estimates of time differences of  $v$  are available.

The crucial point for getting existence for (1) is to establish estimates on these time differences in the absence of a time derivative  $\partial_t v$ . We prove existence of solutions for (1) and convergence of solutions of a corresponding Allen-Cahn system to (1).

[1] A. Bonami, D. Hilhorst and E. Logak: *Modified motion by mean curvature: local existence and uniqueness and qualitative properties*, preprint LMENS 25, (1996)

[2] C. M. Elliott, R. Schätzle and B. Stoth: *Viscosity solutions of a degenerate parabolic elliptic system arising in the mean field theory of superconductivity*, to appear in *Archive of Rational Mechanics and Analysis*, Preprint SFB 256 report no. 498, Bonn, (1998)

[3] Y. Giga, S. Goto and H. Ishii: *Global existence of weak solutions for interface equations coupled with diffusion equations*, *SIAM Journal on Mathematical Analysis*, Vol. 23, No. 4, (1992), pp. 821-835

[4] E. Logak: *Singular limit of reaction-diffusion systems and modified motion by mean curvature*, preprint, (1996)

[5] P. E. Souganidis and P. Soravia: *Phase Field Theory for FitzHugh-Nagumo Type Systems*, *SIAM Journal on Mathematical Analysis*, Vol. 27, (1996), pp. 1341-1359

(joint work with Danielle Hilhorst and Elisabeth Logak)

ALFRED SCHMIDT:

Adaptive finite element method for phase transition problems with convection

Three different problems are discussed, with presentation of (preliminary) numerical results of two dimensional simulations.

(1) The continuous casting Stefan problem, a classical Stefan problem with dominant prescribed convection (constant in space, but time dependent). It models the industrial continuous casting of steel. We present the basic idea of an a posteriori error estimate for the  $L^1(L^1)$  temperature error. It is based on  $L^\infty$  estimates for the corresponding backward parabolic dual problem.

(joint work with Z. Chen (Beijing) and R.H. Nchetto (College Park))

(2) The classical Stefan problem with natural convection in the melt. This is part of a model for the industrial Bridgman growth of semiconductor crystals. The Stefan problem is coupled to the Navier-Stokes equations in Boussinesq approximation in the liquid phase. The time dependent domain and the non-slip boundary condition on the moving interface are implemented in a weak way using a fictitious domain approach. This leads to a saddle point problem, similar to the incompressibility condition. Special preconditioners are needed for efficient solution of the system.

(joint work with K.G. Siebert (Freiburg))

(3) The modified Stefan problem with under-cooling, anisotropic surface tension and natural convection in the melt. It models dendritic growth in a super-cooled liquid under the influence of gravity. Motion of the sharp interface is described by an anisotropic mean curvature flow equation with temperature as driving force.

(joint work with E. Bänsch (Bremen))

GEORG H. SCHMITZ:

Phase-field modelling of solidification phenomena in multiphase systems

The structure of a solid liquid interface is determined by the competition between the ordering influence of structure and the thermal disordering effects. The phase field theory reflects these basic ideas in terms of differential equations, where diffusion, ordering potential and thermodynamic driving force are represented by differential operations of appropriate symmetry. The solution of the phase field equation describes the shape, the curvature and the motion of a diffuse interface, such as the solid-liquid interface in a metallic system. By coupling the phase field equation to the temperature, solute, fluid velocity

and other external fields, this set of equations offers the prospect of being able to perform realistic numerical solidification experiments. In this paper, the history and current state of phase field models and numerical simulations are reviewed. The different aspects of the theory with respect to different coupling fields are demonstrated by relevant examples:

- coupling between multiple phase fields in multi grain growth
- coupling to temperature or solute and dendritic growth
- coupling between two phase fields and solute in peritectic and eutectic solidification
- coupling to velocity in a mush with forced convection.

The presentation will conclude by some considerations about the thermodynamic roots of the double-well potential being used in the phase-field concept.

BEN SCHWEIZER:

The interface between a viscous and inviscid fluid

We study the physical system of two immiscible fluids, one of them viscous and described by the Navier-Stokes equations, the other inviscid and described with Euler equations. The study is motivated by the phenomenon of surface waves on water, generated by wind. The coupling of the free boundary to the fluids is via the geometric conditions and by surface tension. We read the equations as a free boundary problem for one viscous fluid with a nonlocal boundary force, given by the pressure of the Euler-fluid. A decomposition of the pressure distribution identifies two contributions, one being compact and the other with a sign. This observation is used to derive a short time existence result for the two-phase problem. TANG QI:

On thin plate G-L models subject to large parallel applied magnetic field

We discuss the evolutionary G-L superconductivity model on a thin plate domain:  $\Omega = \Omega_0 \times (-\varepsilon, \varepsilon)$  with  $\Omega_0 \subset \mathbb{R}^2$ ,

$$(*) \quad \begin{cases} \frac{\partial \psi}{\partial t} - i\kappa \operatorname{div} A \psi + \left(\frac{i}{\kappa} \nabla + A\right)^2 \psi + (|\psi|^2 - 1)\psi = 0, \\ \frac{\partial A}{\partial t} - \Delta A + \operatorname{Re} \left( \left(\frac{i}{\kappa} \nabla \psi + A\psi\right) \psi^* \right) = \operatorname{curl} H, \\ \frac{\partial \psi}{\partial n} = 0, \quad A \cdot n = 0, \quad \operatorname{curl} A \wedge n = H \wedge n, \\ \psi(x, 0), A(x, 0) = A_0(x). \end{cases}$$

By applying an  $\varepsilon$ -dependent large horizontal applied field of the form

$$H = \left( \frac{H_1}{\varepsilon}, \frac{H_2}{\varepsilon}, H_3 \right),$$

we find that as  $\varepsilon \rightarrow 0$ , the solutions of (\*) converge to the solutions of the following 2-d problem



$$\begin{cases} \frac{\partial \psi}{\partial t} - i\kappa \operatorname{div} A \psi + \left(\frac{i}{\kappa} \nabla + A\right)^2 \psi \\ \quad + \left(|\psi|^2 - 1 + \frac{2}{3}(H_1^2 + H_2^2)\right) \psi = 0 \\ \frac{\partial A}{\partial t} - \Delta A + \operatorname{Re}\left(\frac{i}{\kappa} \nabla \psi + A \psi\right) \psi^* = \operatorname{curl} H_3 \end{cases}$$

where  $A$  is a 2-d vector.

Finally, we investigate the pinning effect of the large horizontal applied field and showed that the effect of  $\left(a(x) = 1 - \frac{2}{3}(H_1^2 + H_2^2)\right) a(x)$  in

$$\int |\nabla \psi|^2 + \frac{1}{2\varepsilon^2} (|\psi|^2 - a(x))^2 dx$$

has similar effect on the location of vortices as the  $a(x)$  in

$$\int a(x) \left( |\nabla \psi|^2 + \frac{1}{2\varepsilon^2} (|\psi|^2 - 1)^2 \right) dx.$$

That is, the vortices are located at  $\{y \in \Omega\}$  such that

$$a(y) = \min_{x \in \Omega} a(x)$$

(joint work with K. H. Hoffmann)

FLORIAN THEIL:

A mathematical model for phase transformation with phase boundary friction

We present a mathematical approach to the theory of martensitic phase transformations in elastic materials. The theory takes into account quasistatic dissipation effects which can prevent phase transformations until a certain energetic threshold is reached. We use the following extremum principle to determine the phase configuration at different moments  $t_k \in \mathbb{R}_\geq$  when the external loading changes:

$$J_{t_k}(u, c_{k-1}, c_k) = \int_{x \in \Omega} W_{c(x)}(\nabla u) + c_k(x) \cdot Dc_{k-1}(x) dx - \langle G_k, u \rangle,$$

where  $u$  is deformation of the loaded body,  $c_{k-1}$  and  $c_k$  represent the phase configuration at time  $t_{k-1}$  and  $t_k$ ,  $D_{ij}$  is the amount of energy necessary to transform a specific volume of phase  $i$  into phase  $j$ ,  $W_{c_i}(\cdot)$  is the strain-energy density function of phase  $i$  and  $G_k$  is a linear functional which represents the external forces at time  $t_k$ . We show that in general minimizing sequences exhibit oscillations thus the functional has to be extended to phase

mixtures. Using results of R. KOHN in homogenisation theory, we shown how this can be done rigorously in the case of two phases, linear elasticity theory and identical elasticity tensors.

A. VISINTIN:

About surface tension and nucleation

Surface tension effects occur in several physical phenomena; in particular, they are responsible for the high *undercooling* required for solid *nucleation* in a purely liquid system.

In a solid-liquid system these effects can be represented by the classical *Gibbs-Thomson law*. Evolution is then represented by the law of *mean curvature flow* with a forcing term:  $av = \theta + c\kappa$  on  $\mathcal{S}$ , where  $v$  is the normal velocity of the interface  $\mathcal{S}$ , and  $a, c$  are positive constants.

Here we want to account not only for smooth surface motion but also for phase *nucleation* and other discontinuities in phase evolution. To that aim we replace the above law by an equation of the form

$$\alpha(v) = \theta + c\kappa \quad \text{on } \mathcal{S}$$

where  $\alpha$  is bounded, monotone, continuous function  $\mathbf{R} \rightarrow \mathbf{R}$  (with  $\alpha'(0) = 1$ ).

A mesoscopic model of phase transition in two-phase systems is then obtained by coupling the latter equation with the energy balance equation.

GEORG SEBASTIAN WEISS:

A homogeneity improvement approach to the one-phase Stefan problem

We present a new approach to semilinear isotropic free boundary problems motivated by the concept of Liapunov stability. The approach is based on an *improvement of the solution's homogeneity* when passing to a smaller scale.

As model problem we consider the one-phase Stefan problem which can near the free boundary be reduced to the stationary obstacle problem. Here we use an *epiperimetric inequality* in order to derive a *decay estimate* for the energy associated with the equation. By a monotonicity formula this leads to the homogeneity improvement and to *unique tangent cones*.

This makes it possible to decompose the free boundary into a relatively open regular set and a singular set on which the solution is twice differentiable.

MATTHIAS WINTER:

Stationary solutions of the Cahn-Hilliard equation: Spikes and bubbles

We study the Cahn-Hilliard equation as a mathematical model for phase transitions in binary materials. The region occupied by the material is supposed to be a bounded smooth domain and we do not assume any symmetries.

Various types of stationary solutions are constructed. These include spike and multiple spike solutions where the location of the spike(s) is at the boundary or in the interior of the domain and interior bubble solutions.

We first use the Liapunov-Schmidt method to reduce the problem to finite dimensions. Then a fixed-point technique or a maximizing procedure is applied to obtain the solutions.

(joint work with J. Wei (Chinese University of Hong Kong))

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