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Phase Transitions

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Abstract. As in the past, the workshop brought together researchers with a background in physics, partial differential equations and continuum mechanics and statistical mechanics. Equilibrium and dynamic phase transitions were discussed. A wide range of systems from solid-solid phase transitions to the quantum Curie Weiss model were considered.

Mathematics Subject Classification (2000): 35, 49, 74, 80, 82.

Introduction by the Organisers

The present workshop was part of a series with the topic of phase transitions, designed especially to bridge the gap in notation and notions of phase transition in different communities, i.e. physics, statistical mechanics, partial differential equations. Judging from the lively discussions it seem to have achieved its goal at least in part. This workshop is the last organized by H. W. Alt, S. Luckhaus, E. Presutti and E.Salje who are handing over to a new team of organizers. An active area of research discussed in many of the talks was the motion of phase interfaces (Dirr, Dreyer, Eck, Esposito, Freistuehler, Melcher, Planes, Zimmer) also in hyperbolic scaling where many questions are still open. The interaction phase interfaces with crystal structure was another topic (Bismayer, Conti, Janssen) for the physics and pde community alike. From quantum statistical mechanics the Curie Weiss model was discussed (Grimmett, Ioffe). Random potentials or environments were an important topic (Bovier, Dirr, Planes , Orlandi) and models of kinetic type played a bigger role than in the previous workshops (Bellettini, Esposito, Marra, Theil). A strength of the workshop were the discussions between the different groups of participants and the organizers feel that in the field of phase transitions this interdisciplinary discourse is particularly important.

Workshop: Phase Transitions

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Abstracts

Γ-convergence and one-dimensional scalar hyperbolic conservation laws

Giovanni Bellettini
(joint work with Lorenzo Bertini, Mauro Mariani, Matteo Novaga)

In this short note we announce in a simplified way some of the results obtained in the joint paper [1] (which is still a work in progress). Let us consider the scalar one-dimensional hyperbolic conservation law

$$u_t + f(u)_x = 0 \tag{1}$$

in $[0,T]\times\mathbb{R}$, and let us confine to uniformly bounded solutions. In order to state the results in a rather simple way, we assume that $f(s) = s^2/2$, even if our theorems are valid under more general assumptions. It is well known that solutions to (1) may develop singularities at finite time, even starting from a smooth initial datum. It is also well established that global existence and uniqueness are recovered by the notion of entropy solution, obtained by enforcing, beside the weak formulation of (1), a further condition, namely $\eta(u)_t + q(u)_x \le 0$ in the sense of distributions, for any convex entropy η, and any $q = q_\eta$ satisfying $q = \int \eta' f'$. Entropy solutions are therefore special distributional solutions (and measure-valued solutions are a larger class of solutions than the distributional ones).
Remarkably, entropy solutions can be obtained as $L_{1,\mathrm{loc}}([0,T]\times\mathbb{R})$- limits, as $\epsilon\to 0$, of the solutions to

$$u_t + f(u)_x = \epsilon u_{xx}. \tag{2}$$

We refer for instance to [2] for the above mentioned definitions and results.
In the recent papers [4], [3], the role of entropic solutions and more generally of distributional solutions is discussed in the context of large deviations. In the framework of Γ-convergence, the observations of [4], [3] can be roughly stated as follows. The idea is to apply the least squares method, namely to define approximating functionals H_ϵ that consist (modulo some rescaling) of the space-time integration of the square of the difference of the left hand side and the right hand side of (1). Solutions to (1) therefore belong to $\{H_\epsilon = 0\}$. Note that, however, H_ϵ is finite also on certain functions which do not solve any sort of pde; indeed $H_\epsilon(u)$ measures the error (or cost) for a function u not to be a solution to (1). It is clear that, in this procedure, beside the definition of the domain of H_ϵ, it is of crucial importance to declare in which norm one wants to measure the cost. For the hyperbolic problem of interest in this note, we will choose essentially the space H^{-1} norm, integrated further in time. Once chosen the functional H_ϵ, the philosophy is then to try to perform the Γ-limit of H_ϵ as $\epsilon\to 0$ (here the choice of the topology is obvioulsy essential) in order to obtain a functional $\mathcal{H}$, expected to vanish only on entropic solutions to (1), and to be (positive and) finite on a rather large class of distributional non-entropic solutions. The value of $\mathcal{H}$ on non-entropic distributional solutions can be considered a measure of how much a distributional

solution to (1) fails to be entropic. The topology for the Γ-limit must be chosen in order to possibly gain at the same time equicoercivity of H_ϵ, which is not, in general, an immediate fact.
Define informally

$$I_\epsilon(u) := \frac{1}{2}\int_0^T \|E\|_{L^2}^2 \, dt,$$

where $E \in L^2([0,T]\times\mathbb{R})$ satisfies

$$u_t + f(u)_x - \epsilon u_{xx} = -E_x, \qquad (t,x) \in (0,T)\times\mathbb{R}.$$

The first result states the equicoercivity and the Γ-convergence of I_ϵ, in a Young measure setting. The limiting functional has an explicit expression and vanishes only on measure-valued solutions to (1).
Let us now rescale the functional I_ϵ and define

$$H_\epsilon := \frac{1}{\epsilon} I_\epsilon.$$

The main result is related to the asymptotic behaviour of the functionals H_ϵ. First we show that H_ϵ are equicoercive (in a suitable topology $\mathcal{T}$). Then we show that the $\Gamma(\mathcal{T})$-$\liminf_{\epsilon\to 0}$ of H_ϵ is larger than or equal to the functional $\mathcal{H}$ defined as follows. If u is not a distributional solution to (1) then $\mathcal{H}(u) = +\infty$, otherwise $\mathcal{H}(u)$ is the total variation of the positive part of the entropy production $h(u)_t + g(u)_x$, where $h(s) = s^2/2$ and $g(s) = s^3/3$. Note that $\mathcal{H}$ vanishes only on entropic solutions to (1). Finally, we show that, for any function u in a class X of "well-behaved" functions, the $\Gamma(\mathcal{T})$-$\limsup_{\epsilon\to 0}$ of H_ϵ at u is smaller than or equal to $\mathcal{H}(u)$. The Γ-convergence result is at the moment not complete, since we miss the proof that given any function u in the domain of $\mathcal{H}$, there exists a sequence of functions $u_\epsilon \in X$ converging to u with respect to $\mathcal{T}$, and such that $\mathcal{H}(u_\epsilon)$ converges to $\mathcal{H}(u)$ as $\epsilon \to 0$. In particular, we miss the $\mathcal{T}$-density of X in the domain of $\mathcal{H}$ (which may strictly contain the space of functions of bounded variation).
From the variational point of view, it is worth noticing that, even ignoring the definitions of entropic solution and of distributional solution of (1), such notions could be in principle recovered a posteriori by identifying the zero level set and the domain of $\mathcal{H}$.

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Ferroelastic domains in lead phosphate-type crystals

U. Bismayer

Lead phosphate $Pb_3(PO_4)_2$ and isostructural mixed crystals of the palmierite-type undergoe an improper ferroelastic phase transformation from a rhombohedral paraelastic high temperature phase $R\overline{3}m$ to a monoclinic ferroelastic low temperature phase C2/c. The order parameter transforms according to the three-dimensional irreducible representation of a critical point at the boundary of the Brillouinzone. Salje and Devarajan [1] described the transformation in terms of a three-states Potts model which could explain the persistence of monoclinic signals above the ferroelastic transition point. These signals are due to small Pb-displacements inside dynamic monoclinic clusters in the rhombohedral matrix. The corresponding Hamiltonian can be separated in an orientational term with components (Q_1, Q_2) and a Landau potential in Q_3 described by the effective Gibbs free energy [2]

$$\Theta' = \frac{\alpha'}{2}Q_3^2 + \frac{\beta}{4}Q_3^4 + \frac{\gamma}{6}Q_3^6 \tag{1}$$

$$\Theta'' = (\frac{\alpha}{2} + L_3M^2)(Q_1^2 + Q_2^2) + L_2(Q_1^2 + Q_2^2)^2 + wQ_1(Q_2^2 - \frac{1}{3}Q_1^2) \tag{2}$$

with

$$M = \langle Q_3 \rangle, w = \frac{1}{\sqrt{2}}L_4\langle Q_3 \rangle \tag{3}$$

and constants L_i.

At the ferroelastic transformation point the rhombohedral symmetry of the matrix is broken, preferential orientations of the binary axis are chosen along three symmetry-allowed directions (Fig. 1) and static macroscopic ferroelastic domais appear. Following general group theoretical considerations there are twelve $C12/c1$ subgroups of $R\overline{3}m$ of index 6 with doubled number of atoms in the unit cells. The $C12/c1$ subgroups are distributed into four conjugacy classes of three subgroups each. They correspond to three orientational domains. Six of the subgroups are derived via two sub-chains with an intermediate subgroup $C12/m1$ and $R\overline{3}c$, and can be associated with the one-arm k-vector star $T(1/2,\ 1/2,\ 1/2)$ of $R\overline{3}m$. The other six subgroups of $C12/c1$ which are derived from the subgroup chain $R\overline{3}m > C12/m1 > C12/c1$ are relevant for the transformation observed in lead phosphate. The corresponding symmetry break is described by the tree-arm k-vector star $L(1/2,0,0;\ 0,1/2,0;\ 0,0,1/2)$. The three maximal *translationengleiche* subgroups $[C12/m1]_k$ (k=1,2,3) of $R\overline{3}m$ correspond to three allowed orientations of the monoklinic axes with respect to the rombohedral high-symmetry group. Resulting ferroelastic domains can be seen between crossed polarisors under an optical microscope (Fig. 2). The splitting of the Wyckoff positions for $Pb_3(PO_4)_2$ and the symmetry mode analysis has been described by Paulmann et al. [3] who showed that the secondary modes are invariant with respect to $R\overline{3}m$ and that the

symmetry break from rhombohedral to monoclinic by the primary mode involves the displacement of Pb(1) atoms in Wyckoff position 3a.

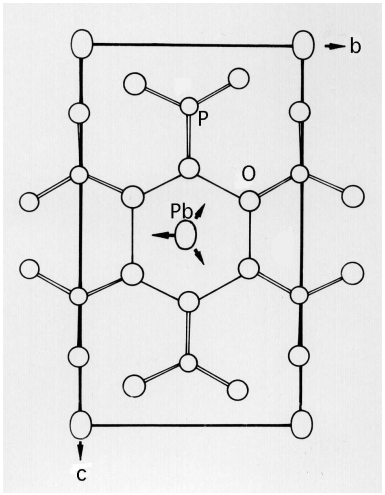

FIGURE 1. bc-plane of the lead phosphate structure with three symmetry equivalent Pb displacement directions

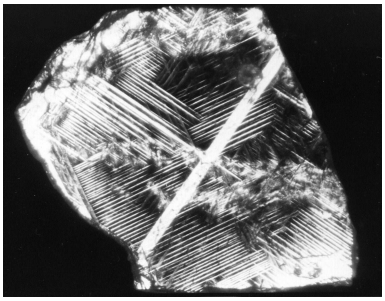

FIGURE 2. Ferroelastic domains in lead phosphate observed under the optical microscope (area of 2 x 1.5 mm)

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Ageing in spin glass models at intermediate time scales: Universality of the trap model

Anton Bovier
(joint work with G. Ben Arous,J. Černý)

Aging has become one of the main paradigms to describe the long-time behavior of complex and/or disordered systems. Systems that have strongly motivated this research are *spin glasses*. The theoretical modeling of aging phenomena took a major leap with the introduction of so-called *trap models* by Bouchaud and Dean in the early 1990'ies [BD95] (see [BCKM98] for a review). These models reproduce the characteristic power law behavior seen experimentally while being sufficiently simple to allow for detailed analytical treatment. While trap models are heuristically motivated to capture the behavior of the dynamics of spin glass models, there is no clear theoretical, let alone mathematical derivation of these from an underlying spin-glass dynamics. The first attempt to establish such a connection was made in [BBG03a, BBG03b] where it was shown that starting from a particular Glauber dynamics of the Random Energy Model (REM), at low temperatures and at the time scale slightly shorter than the equilibration time of the dynamics, the aging of the time-time correlation function of the dynamics converged to that given by Bouchaud's REM-like trap model.

On the other hand, in a series of papers [BČ05, BČM06, BČ07a, BČ07b] a systematic investigation of a variety of trap models was initiated. In this process, it emerged that there appears to be an almost universal aging mechanism based on α-stable subordinators that governs aging in most of the trap models. It was also shown that the same feature holds for the dynamics of the REM at shorter time scales. For a general review on trap models see [BČ06].

In all models considered so far, however, the random variables describing the quenched disorder were considered to be independent, be it in the REM or in the trap models. Here we report first results obtained in [BBČ07] that show that the same mechanisms are at work in correlated spin glasses.

Let us describe the class of models we are considering. Our state spaces will be the N-dimensional hypercube, $\mathcal{S}_N \equiv \{-1,1\}^N$. $R_N : \mathcal{S}_N \times \mathcal{S}_N \to [-1,1]$ denotes as usual the normalized overlap, $R_N(\sigma,\tau) \equiv N^{-1}\sum_{i=1}^N \sigma_i\tau_i$. The Hamiltonian of the p-spin SK-model is defined as $\sqrt{N}H_N$, where $H_N : \mathcal{S}_N \to \mathbb{R}$ is the centered normal process indexed by $\mathcal{S}_N$ with covariance

$$\mathbb{E}[H_N(\sigma)H_N(\tau)] = R_N(\sigma,\tau)^p, \tag{1}$$

and $p \in \mathbb{N}$, $p > 2$.

We define the classical trap-model dynamics as a nearest neighbor continuous time Markov chain $\sigma_N(\cdot)$ on $\mathcal{S}_N$ with transition rates

$$w_N(\sigma,\tau) = \begin{cases} N^{-1}e^{-\beta\sqrt{N}H_N(\sigma)}, & \text{if } \mathrm{dist}(\sigma,\tau) = 1, \\ 0, & \text{otherwise;} \end{cases} \tag{2}$$

here $\mathrm{dist}(\cdot,\cdot)$ is the Hamming distance.

This dynamics is a time change of a simple random walk on $\mathcal{S}_N$: Let $Y_N(k) \in \mathcal{S}_N$ be the simple unbiased random walk (SRW) on $\mathcal{S}_N$. Define the *clock-process* by

$$S_N(k) = \sum_{i=0}^{k-1} e_i \exp\left\{\beta\sqrt{N} H_N\big(Y_N(i)\big)\right\}, \tag{3}$$

where $\{e_i, i \in \mathbb{N}\}$ are i.i.d. standard exponential random variables. Then the process $\sigma_N(\cdot)$ can be written as

$$\sigma_N(t) \equiv Y_N(S_N^{-1}(t)). \tag{4}$$

The main result on the dynamics will be the following theorem that provides the asymptotic behavior of the clock process.

Theorem 1. *There exists a function $\zeta(p)$ such that for all $p \geq 3$ and γ satisfying*

$$0 < \gamma < \min\left(\beta^2, \zeta(p)\beta\right), \tag{5}$$

under the conditional distribution $\mathbb{P}[\cdot|\mathcal{Y}]$ the law of the stochastic process

$$\bar{S}_N(t) = e^{-\gamma N} S_N\big(\lfloor tN^{1/2} e^{N\gamma^2/2\beta^2} \rfloor\big), \qquad t \geq 0, \tag{6}$$

defined on the the space of càdlàg functions equipped with the Skorokhod M_1-topology, converges, $\mathcal{Y}$-a.s., to the law of γ/β^2-stable subordinator $V_{\gamma/\beta^2}(Kt), t \geq 0$, where K is a positive constant depending on γ, β and p.

Moreover, the function $\zeta(p)$ is increasing and it satisfies

$$\zeta(3) \simeq 1.0291 \qquad \text{and} \qquad \lim_{p\to\infty} \zeta(p) = \sqrt{2\log 2}. \tag{7}$$

To control the behaviour of spin-spin correlation functions that are commonly used to characterize aging, we need to know more on how these jumps occur at finite N. What we will show, is that if we the slightly coarse-grain the process $\bar{S}_N$ over blocks of size $o(N)$, the rescaled process does converge in the J_1-topology. What this says, is that the jumps of the limiting process are compounded by smaller jumps that are made over $\leq o(N)$ steps of the SRW. In other words, the jumps of the limiting process come from waiting times accumulated in one slightly extended trap, and during this entire time only a negligible fraction of the spins are flipped. That will imply the following aging result.

Theorem 2. *Let $A_N^\varepsilon(t,s)$ be the event defined by*

$$A_N^\varepsilon(t,s) = \left\{R_N\big(\sigma_N\big(te^{\gamma N}\big), \sigma_N\big((t+s)e^{\gamma N}\big)\big) \geq 1-\varepsilon\right\}. \tag{8}$$

Then, under the hypothesis of Theorem 1, for all $\varepsilon \in (0,1)$, $t > 0$ and $s > 0$,

$$\lim_{N\to\infty} \mathbb{P}[A_N^\varepsilon(t,s)] = \frac{\sin\alpha\pi}{\pi} \int_0^{t/(t+s)} u^{\alpha-1}(1-u)^{-\alpha}\,\mathrm{d}u. \tag{9}$$

Let us discuss the meaning of these results. $e^{\gamma N}$ is the time-scale at which we want to observe the process. According to Theorem 1, at this time the random walk will make of the order of $N^{1/2}e^{N\gamma^2/2\beta^2} \ll e^{\gamma N}$ steps. Since this number is

also much smaller than 2^N (as follows from (7)), the random walk will essentially visit that number of sites.

If the random process H_N was i.i.d., then the maximum of H_N along the trajectory would be $\left(2\ln(N^{1/2}e^{N\gamma^2/2\beta^2})\right)^{1/2} \sim N^{1/2}\gamma/\beta$, and the time spent in that site would be of order $e^{\gamma N}$. Since Theorem 1 holds also in the i.i.d. case, that is in the REM (see [BČ07a]), the time spent in the maximum is comparable to the total time and the convergence to the α-stable subordinator implies that the total accumulated time is composed of pieces of order $e^{\gamma N}$ that are collected along the trajectory. In fact, each jump of the subordinator corresponds to one visit to a site that has waiting times of that order. In a common metaphor, the sites are referred to as traps and the mean waiting times as their depths.

The theorem in the general case states that in the p-spin model, the same is essentially true. The difference will be that the traps here will not consist of a single site, but consist of a deep valley (along the trajectory) whose bottom that has approximately the same energy as in the i.i.d. case and whose shape and width we will be able to describe quite precisely. Remarkably, the number of sites contributing significantly to the residence time in the valley is essentially finite, and different valleys are statistically independent.

The proof of Theorem 1 relies on the combination of detailed information on the properties of simple random walk on the hypercube and comparison of the process H_N on the trajectory of the SRW to a simpler Gaussian process using interpolation techniques.

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Domain structures in solid-solid phase transitions

Sergio Conti

The variational modeling of solid-solid phase transition is based on functionals of the form

$$I_0[u] = \int_\Omega W(\nabla u) dx \,,$$

where $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}^n$ represents the elastic deformation; a typical form for the energy density W is

$$W(F) = \mathrm{dist}^2(F, K) = \inf\{|F - G|^2 : G \in K\} \,.$$

The set of energy-minimizing deformation gradients $K \subset \mathbb{R}^{n\times n}$ depends on the specific phase transformation considered. For cubic-tetragonal phase transitions in three dimensions K equals $K_3 = SO(3)\{U_1, U_2, U_3\}$, where the U_i are the three diagonal matrices with eigenvalues $(\lambda, \lambda, \lambda^{-2})$, $\lambda \neq 1$ being a positive parameter. In two dimensions one uses $K_2 = SO(2)\{U_1, U_2\}$, with eigenvalues λ and $1/\lambda$.

The theory of convex integration permits to find deformations u such that $W(\nabla u) = 0$ pointwise. The following result was obtained by Müller and Šverák [14] in two dimensions, and later generalized to three dimensions in [6, 3].

Theorem 3 (From [14, 6, 3])**.** *Let $n = 2$ or 3. There is $r > 0$ such that, for all matrices $F \in \mathbb{R}^{n\times n}$ with $\det F = 1$ and $|F - \mathrm{Id}| < r$, and all open sets $\Omega \subset \mathbb{R}^n$, we can find $u \in W^{1,\infty}(\Omega; \mathbb{R}^n)$ such that $u(x) = Fx$ for $x \in \partial\Omega$ and $\nabla u \in K_n$ a.e. on Ω.*

These deformations are however unphysical since they have very low regularity (precisely, u is Lipschitz but nowhere C^1, and its gradient does not have bounded variation, see [7, 9]).

One is therefore lead to singularly perturbed functionals which include terms penalizing interfaces, of the form

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

ε being a (small) positive parameter. A first step toward an understanding of the behavior of such functionals is the analysis of the scaling behavior for small ε; in some cases a finer Γ-convergence result has been obtained, see, e.g., [5, 4].

We focus here on the two-dimensional situation; after a change of variables we can assume that

$$K = SO(2) \left\{ \begin{pmatrix} 1 & \eta \\ 0 & 1 \end{pmatrix} , \begin{pmatrix} 1 & -\eta \\ 0 & 1 \end{pmatrix} \right\} \tag{2}$$

where $\eta \neq 0$ is a parameter, and assume as boundary values $u(x) = x$ for $x \in \partial\Omega$. The domain Ω can for simplicity be taken to be the unit square. It has recently been shown by Lorent [13] that the scaling behavior of the minimum of I_ε over Sobolev functions is equivalent to the one of the unperturbed functional I_0 over appropriate discretized functions constructed on a grid of mesh size proportional to ε, hence studying I_ε also leads to results on finite-element discretizations.

A scalar simplification of this problem was considered by Kohn and Müller in 1992-94, see [10, 11]. Precisely, they proposed the functional

$$J_\varepsilon[v] = \begin{cases} \int_\Omega (D_1 v)^2 dx + \varepsilon \int_\Omega |D_2 D_2 v| & \text{if } |D_2 v| = 1 \text{ a.e.,} \\ \infty & \text{otherwise} \end{cases}$$

(the second derivative is here understood distributionally). They have shown that there is $c > 0$ such that

$$\frac{1}{c}\varepsilon^{2/3} \le \min\{J_\varepsilon[v] : v = 0 \text{ on } \partial\Omega\} \le c\varepsilon^{2/3}\,. \tag{3}$$

The parallel between J_ε and I_ε can be heuristically analyzed by considering the relation $u(x) \simeq x + \eta v(x) e_1$ between the corresponding test functions.

We consider here the full vectorial problem, and obtain a similar result.

Theorem 4 (From [1]). *Let $n = 2$, I_ε and K be as in (1) and (2). Then there is $c > 0$ such that, for all $\varepsilon \in (0, 1)$,*

$$\frac{1}{c}\varepsilon^{2/3} \le \min\{I_\varepsilon[u] : u(x) = x \text{ on } \partial\Omega\} \le c\varepsilon^{2/3}\,. \tag{4}$$

The key idea in proving the upper bound is to take a mollification of a vectorial extension of the construction from [10, 11], see [1]. The lower bound requires instead appropriate rigidity estimates, which can deal with the two-well structure of K. A first two-well rigidity result was obtained by Lorent [12], who has shown that there are constants $c, \gamma, \theta > 0$ such that if $\int_{B_2} |D^2 u| < \theta$ (and some other assumptions hold) then

$$\min_{F \in K} \int_{B_1} \operatorname{dist}(\nabla u, SO(2)F)\, dx \le c \left(\int_{B_2} \operatorname{dist}(\nabla u, K)\, dx \right)^\gamma . \tag{5}$$

It was then shown in [4] that the same holds with the optimal exponent $\gamma = 1$. Combining (5) with the quantitative Friesecke-James-Müller rigidity estimate [8] permits the use of the strategy developed in [2] to obtain a lower bound for I_ε.

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Interfaces in a Heterogeneous Environment

Nicolas Dirr

1. Introduction

I am interested in the macroscopic behavior of gradient flow models which are perturbed on a smaller scale by periodic or random heterogeneities. This interest is motivated by models for material behavior in the overdamped limit, where often the time evolution is modeled by a partial differential equation. These models should incorporate heterogeneities, which may arise from the periodic structure of the material or a substrate, or they model impurities which are present in the material on a very fine scale. These heterogeneities create a very oscillatory energy landscape and make the qualitative analysis of the dynamics very challenging. In particular, the large scale limit of the energy, obtained e.g. by the means of Γ-convergence, (see e.g. [2]) and the large-scale limit of the gradient flow dynamics may not commute, i.e. the gradient flow of the limiting energy is *not* the scaling limit of the gradient flows, because the gradient flow gets stuck in the local minima created by the heterogeneities, which are averaged out by the Γ-limit. (For more details see [3].)

Motivated by the evolution of phase boundaries (e.g. in ferromagnetic materials), I choose as energy for the gradient flow models the interfacial energy (area of a hypersurface). In other words, I consider models which capture the interplay of

- the interfacial energy;
- time-independent random and/or deterministic inhomogeneities on a very small spatial scale;

A simple, but due to the interaction of nonlinearities and heterogeneities already quite challenging model is *mean curvature flow with periodic forcing,* i.e. the geometric evolution equation

$$V_x = \kappa_x + f(x) + F, \tag{1}$$

where V_x is the normal velocity and κ_x the mean curvature of the interface $\Sigma(t)$ at a point $x \in \mathbb{R}^n \cap \Sigma(t)$, and F a constant driving field.

The question of interest is the *effective velocity* on a large space-time scale. This can be phrased as follows: Is there for any direction $\nu \in S^{n-1}$ a speed c_ν such that a solution starting from a plane with normal ν stays within bounded distance from a plane with that normal which moves with normal velocity c_ν?

Due to the comparison principle it is sufficient to find special solutions with this property. We look for so-called pulsating wave solutions, i.e. solutions for which a spatial translation that keeps the periodic environment invariant (lattice translation) corresponds to a translation in time.

The main technical difficulty (next to the nonlinear nature of the mean curvature flow) lies in the fact that we allow $f(x) + F$ to change sign. For a forcing which is *positive* and satisfies additional technical conditions, this problem has been solved by P.L. Lions and P.E. Souganidis within the framework of homogenization for viscosity solutions of fully nonlinear pdes, see [4]. Note that the corresponding homogenization problem becomes "singular" in the sense that the highest order term (the mean curvature operator) is multiplied by the small parameter $\epsilon \to 0$: The ϵ-problem is $V = \epsilon\kappa + f(x/\epsilon)$, while the homogenized problem is $V = c_\nu$. If the forcing changes sign, then certain Lipschitz estimates are no longer available.

1. Pulsating Waves for a semilinear PDE (Joint work with Nung Kwan Yip)

We first considered a slightly simplified situation. We assume that the interface is a graph $(x, u(x,t))$ over a coordinate plane (i.e. ν is a unit vector) and make for small gradients the following (heuristic) approximation of the equation: $u(x,t)$: $\mathbb{R}^n \times \mathbb{R}_+ \to \mathbb{R}$ periodic in x,

$$u_t = \Delta u + f(x,u) + F, \tag{2}$$

$f(\cdot,\cdot)$ is 1-periodic in *both* variables, bounded, mean zero, and $F \geq 0$ is an external driving force. We show (see [3]): There exists $F_* > 0$ such that for any $0 \leq F \leq F_*$ there exists a periodic stationary solution of (2), for $F > F_*$, there exist *pulsating wave solutions* $U_F(x,t)$ with velocity V_F, i.e. $U_F(\cdot, t + 1/V_F) = U_F(\cdot,t) + 1$. For a large class of $f(x,u)$ we show that the velocity of the pulsating wave near the critical forcing scales like $[(F - F_*)_+]^{\frac{1}{2}}$, for details see [3].

2. Pulsating Waves for forced mean curvature flow with weak forcing (Joint work with Georgia Karali and Nung Kwan Yip)

Forced mean curvature flow is degenerate parabolic, hence it may develop singularities in finite time and need not stay a graph over a plane, even if the initial datum is exactly that plane. In order to stay in a parabolic setting, we require that the forcing $f(x) + F$ is sufficiently small in C^1, but we do not require that $f(x) + F$ has a sign.

Under this assumption we are able to show that for any normal direction ν there exists a speed c_ν and a number $D > 0$ such that a solution of (1) starting from a plane with normal ν is a graph over that plane for all positive times, and this graph has a distance of at most D from a plane with normal ν moving with

normal velocity c_ν. We use geometric arguments based on ideas of L. Caffarelli and R. de la Llave, [1]

If $c_\nu \neq 0$, we show that pulsating waves exist. (Work in preparation).

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Modelling of Nucleation Phenomena

Wolfgang Dreyer

(joint work with Frank Duderstadt, Margarita Naldzhieva)

1. Introduction This is a study on various aspects of nucleation and evolution of precipitates in a given surrounding.

2. The Becker-Döring (BD) model. The BD model relies on the BD process, which considers a condensation reaction, where a droplet with α molecules grows by incorporation of a monomer from the surrounding, and an evaporation reaction where a droplet shrinks by emitting a monomer into the surrounding. Other processes, like the appearance of a droplet with $\alpha+\beta$ molecules due to a reaction of a droplet with $\alpha > 1$ molecules with another droplet with $\beta > 1$ molecules, are not considered within the BD process.

The central quantity of the BD model is the function $Z(t,\alpha) \geq 0$, which give at any time $t \geq 0$ the number of droplets with α molecules. The number of monomers is included here, and it is given by $Z(t,1)$.

The evolution of $Z(t,\alpha)$ is determined by a system of ordinary differential equations, that we call nowadays the BD system. It reads for $\alpha \in \{2,...,\nu\}$

$$\frac{\partial Z(t,\alpha)}{\partial t} = J_{\alpha-1} - J_\alpha \quad \text{with} \quad J_\alpha = \Gamma^{\mathrm{C}}_\alpha Z(t,\alpha) - \Gamma^{\mathrm{E}}_{\alpha+1} Z(t,\alpha+1). \tag{1}$$

Here $\nu < \infty$ is an artificial number, which restricts the maximal size of a droplet. Obviously, we are finally interested in the limit $\nu \to \infty$. The evolution law for the number of monomers $Z(t,1)$ results from the conservation of the total number of molecules $N = \sum_{a=1}^{\nu} \alpha Z(t,\alpha)$ and can be written as

$$\frac{\partial Z(t,1)}{\partial t} = -J_1 - \sum_{a=1}^{\nu} J_\alpha. \tag{2}$$

The condensation rate $\Gamma_\alpha^{\mathrm{C}}$ and the evaporation rate $\Gamma_\alpha^{\mathrm{E}}$ give the number of reactions per second, and they must be determined by constitutive laws, which were derived in [1].
Within the described setting, there are various models available in the literature. These models mainly differ by different transition rates. Ball, Carr and Penrose, [2], achieved several important mathematical results for a certain class of transition rates. In particular we mention here Penrose's study, [3], on the long time behaviour of a many droplet system and its approach to the Lifshitz/Slyosov/Wagner (LSW) theory in a certain scaling limit. Penrose reasonings were rigorously proved by B. Niethammer in 2002, [4].

The transition rates of the current study rely on the observation by Dreyer and Duderstadt, [1], that the ratio $\Gamma_{\alpha+1}^{\mathrm{E}}/\Gamma_\alpha^{\mathrm{C}}$ is restricted by the 2^{nd} *law of thermodynamics* according to

$$\frac{\Gamma_{\alpha+1}^{\mathrm{E}}}{\Gamma_\alpha^{\mathrm{C}}} = \frac{\sum_{\beta=1}^{\nu} Z(t,\beta)}{Z(t,1} \exp \frac{A_{\alpha+1} - A_\alpha}{kT}. \tag{3}$$

The newly introduced quantities A_α are available free energies of a system that contains a single droplet with α molecules in a given surrounding, which is either pressure or volume controlled. In the Dreyer/Duderstadt model, the condensation rate $\Gamma_\alpha^{\mathrm{C}}$ is independent of $Z(t,\alpha)$ for fixed external pressure. Thus the nonlinearity of the BD system is due to the evaporation rates. The mathematical treatment of this model is found to be in [5].

The available free energy $\mathcal{A}$ of the many droplet system is given by

$$\mathcal{A} = \sum_{\alpha=1}^{\nu} Z(t,\alpha) A_\alpha + kT \sum_{\beta=1}^{\nu} Z(t,\alpha) \ln \left(\frac{Z(t,\alpha)}{\sum_{\beta=1}^{\nu} Z(t,\beta)}\right), \tag{4}$$

and $\mathcal{A}$ is identified as the Lyapunov function of the BD model, i.e. $d\mathcal{A}/dt \leq 0$.

3. Evolution of a single droplet system at fixed external pressure. Thus the physics of nucleation and evolution of droplets and bubbles in a given surrounding may be encoded in the available free energy A_α of a system with a single precipitate. In its domain of definition A_α has an inner maximum and minima which, depending on the boundary conditions, may be found on the boundary or in the interior of the domain. The height and the location of the maximum determines the nucleation regime, whereas the locations of the minima control the subsequent evolution.

The most simple description of the evolution of a single precipitate ignores its coupling to a changing temperature in the vicinity of the phase boundary and a flow field, which is due to the differences of the different mass densities of the evolving adjacent phases. As an example to illustrate the influence of a flow field at constant temperature we consider an evolving spherical bubble of vapour with homogeneous mass density within a large domain of an incompressible liquid, so that we meet radial symmetry of the process. Mass and momentum balances within the bulk phases and across the interface, and a kinetic relation, which relates the change of the bubble mass to the differences of the Gibbs free energies

across the the interface, yield 3 nonlinear ODE's for the bubble mass, radius and interfacial speed. Figure 1 shows the evolution of the bubble radius without (left) and with the incorporation (middle) of the flow field. The right graph combines the both cases. We observe a drastic slow down of the interfacial evolution and conclude that simplified models may fail to describe the process appropriately.

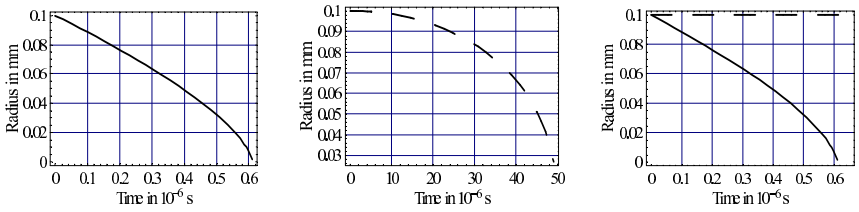

FIGURE 1. Evolution of a bubble in a liquid for 2 different cases

3. From Becker-Döring to Fokker-Planck. From a numerical point of view, a BD system containing more than, say, 50000 ODEs is hard to control. For this reason, the discrete description of nucleation and evolution of droplets will be stopped for some sufficient large ν, which is the number of molecules in the largest droplet within the discrete setting. For larger droplets with $\alpha > \nu$ we seek for a continuous description by a single PDE for a continuous variable x which is the continuous analog of the discrete particle number α. Thus we expect for $\alpha > \nu$ the transition

$$(5)\quad Z(t,\alpha) \quad \to \quad f(t,x) \quad \text{so that} \quad \frac{\partial Z(t,\alpha)}{\partial t} = J_{\alpha-1} - J_\alpha \quad \to \quad \frac{\partial f}{\partial t} = -\frac{\partial J}{\partial x}.$$

This transition confronts us with the problem how to define appropriately the the continuous flux J. From the literature we find various suggestions. The following examples are due to Frenkel and Goodrich, respectively.

$$(6)\quad J = -\frac{\partial}{\partial x}(\Gamma^C f) + (\Gamma^C - \Gamma^E)f \quad \text{and} \quad J = \frac{1}{2}\frac{\partial}{\partial x}((\Gamma^C + \Gamma^E)f) + (\Gamma^C - \Gamma^E)f.$$

These differences are due to different substitutions of finite differences by derivatives, and in any case the resulting PDE is of *Fokker-Planck* type. However, it turns out that the chosen form of J has an enormous impact on the dynamical behaviour as well as on the possible equilibria. Next we give a suggestion made by D. Duncan, which reads

$$(7)\qquad J = -\frac{\partial f}{\partial x} + (\frac{\partial A}{\partial x} + \ln(\lambda(t)))f,$$

where $\lambda(t)$ depends nonlocally on $f(t,\cdot)$. We have shown that Duncan's flux is necessary so that the available free energy of the mixed BD–FP system,

$$\begin{aligned}(8)\qquad \mathcal{A} &= kT\sum_{\alpha=1}^{\nu} Z(t,\alpha)\ln\Big(\frac{Z(t,\alpha)}{\exp\big(\frac{-A_\alpha}{kT}\big)\sum_{\beta=1}^{\nu} Z(t,\beta)}\Big)\\ &\quad + kT\int_{\nu+1}^{\infty} f(t,x)\ln\Big(\frac{f(t,x)}{\exp\big(\frac{-A(x)}{kT}\big)\int_{\nu+1}^{\infty} f(t,y)dy}\Big)dx,\end{aligned}$$

satisfies

$$(9)\qquad \frac{d\mathcal{A}}{dt} \le 0.$$

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A two–scale model for liquid phase epitaxy

Christof Eck

(joint work with Heike Emmerich)

Epitaxy is a technique to produce thin solid films by the deposition of single atoms. In liquid phase epitaxy the atoms are solved in a liquid and transported to the interface by diffusion and convection. There they may attach to the solid film, where they may diffuse until they reach an existing monoatomar step and incorporate to the solid phase. The monoatomar steps can be created by nucleation or they are triggered by existing dislocations.

We consider a model for liquid phase epitaxy that combines standard differential equations for fluid flow and solute transport in the liquid with a Burton–Cabrera–Frank model (BCF–model) for the growth of the solid film. The BCF model [1] combines a continuum mechanical description for the diffusion process of the attached atoms on the surface in horizontal directions and an atomistic description of the single atom layers in vertical direction. The boundaries of the monoatomar steps are modeled as a free surface. In the case of thermodynamic equilibrium, the conditions at the free surface are similar to those of a Stefan–problem with Gibbs–Thomson effect. The models are coupled by equations describing the conservation of mass via a suitable exchange of mass between liquid and solid phase.

In many experiments one observes characteristic microstructures of e.g step–wise, pyramidal or spiral morphology. In order to derive a model that is applicable for a very small scale of this microstructure while still accounting for the macroscopic range of the transport processes in the liquid, we perform a homogenization limit $\varepsilon \to 0$ for a microscale parameter ε. This is done for suitable scalings of the parameters in the model that basically describe a diffusion length of scale ε for the surface diffusivity and a dilute solution in the liquid. The corresponding two–scale limit consists of a macroscopic Navier–Stokes system and a macroscopic convection–diffusion–equation, coupled to microscopic cell problems of BCF-type for the evolution of single microstructure elements. The existence of solutions to the two–scale model is proved, and an estimate for the model error is derived. It is proved that the difference between the solution of the original problem for scale ε and a macroscopic reconstruction of the solution of the two–scale model scales as $\varepsilon^{1/2}$, see [2].

Elastic deformations of the solid phase can be included to the model by adding a system of equations for static linear elasticity. This system is coupled to the Navier–Stokes system in the liquid phase by conditions describing the conservation of mass and the equilibrium of forces. Boundary conditions for the elasticity equations model possible misfit strains at the boundary between the substrate and the solid phase. A formal two–scale expansion under the assumption that the elastic displacement scales proportional to ε again leads to a two–scale model. The elasticity equations enter the microscopic equations while the two–scale limit of the Navier–Stokes system leads to a microscopic Stokes system and a macroscopic Navier–Stokes System.

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Kinetic description of phase transitions in binary fluids

Raffaele Esposito

The problem of the phase transitions is a relatively well understood issue in the framework of the Equilibrium Statistical Mechanics. Much less is known from a dynamical point of view. Of course, a better understanding of dynamical aspects of phase transitions is desirable both for theoretical and practical reasons, but the present state of the theory does not allow a satisfactory dynamical analysis at microscopic level.

It is then natural to try to construct models at some mesoscopic scale where it is possible to analyze in a mathematically rigorous way the dynamics of phase transitions. The obvious candidate for such a model is a kinetic gas. The classical Boltzmann equation however only describes ideal gases which do not undergo any phase transition. As in Equilibrium Statistical Mechanics, it is possible to get a model exhibiting phase transition by adding suitable weak long range interactions (Kac potentials) which in kinetic theory give rise to Vlasov-type self consistent forces. The simplest model one could consider is then a rarefied Boltzmann gas with an extra long range attraction. This model however is not stable because nothing would prevent its collapse and in order to stabilize it one should include some close packing condition, as in the van der Waals gas. Such a mechanism is not easy to model in a natural way in the kinetic framework.

A slightly more complex model, but better suited to our purposes, is obtained by considering a binary gas composed of two species of molecules (for simplicity with the same mass) colliding regardless of the species, but also interacting via a weak repulsive long range force between molecules of different species. It is intuitively clear that in this model, at sufficiently low temperature, the molecules of the two species prefer to stay away from each other, so that the system undergoes a *segregation* phase transition. This model is the analog of a binary alloys, but with extra effects due to momentum and energy transport. It has been introduced in [1] where it has been studies via Monte Carlo simulations.

The equations describing the model are given in terms of the probability densities on the phase space for the two species, $f_i(x, v, t)$, $i = 1, 2$, $x \in \Omega \subset \mathbb{R}^d$ being the position, $v \in \mathbb{R}^3$ the velocity and $t \geq 0$ the time:

$$\partial_t f_1 + v \cdot \nabla_x f_1 + F_1 \cdot \nabla_v f_1 = J(f_1, f_1) + J(f_1, f_2)$$

$$\partial_t f_2 + v \cdot \nabla_x f_2 + F_2 \cdot \nabla_v f_2 = J(f_2, f_1) + J(f_2, f_1)$$

where the self-consistent forces $F_i, i = 1, 2$, are

$$F_i(x, t) = -\nabla_x \int_\Omega dx' U(|x - x'|) \int_{\mathbb{R}^3} \mathrm{d}v f_{i+1(\mathrm{mod}\ 2)}(x', v, t)$$

and $J(f, g)$ is the usual (non symmetric) Boltzmann collision operator.

The question of the derivation of the model from a microscopic dynamics in some scaling limit has been addressed in [2], where it is discussed formally. The rigorous validity is an open problem, due to the topology mismatch between the proofs of validity of the Boltzmann and Vlasov equations.

Entropy arguments show that the equilibrium solutions are given by Maxwellians $f_i(x, v) = \rho_i(x) \dfrac{\mathrm{e}^{-v^2/2T}}{(2\pi T)^{3/2}}$ with zero average, the same temperature and densities possibly depending on x and satisfying the equations:

$$T \log \rho_i(x) + \int_\Omega dx' U(|x - x'|) \rho_{i+1(\mathrm{mod}\ 2)}(x') = C_i.$$

Above condition turn out to be the Euler-Lagrange equations for the minimization problem to the free energy functional

$$\mathcal{F}(\rho_1,\rho_2) = T\int_\Omega dx(\rho_1\log\rho_1+\rho_2\log\rho_2)+\int_{\Omega\times\Omega} dxdx' U(|x-x'|)\rho_1(x)\rho_2(x').$$

This is the starting point of the analysis in [3], where, in a slightly more general setup and with the assumption that Ω be a d-dimensional torus, we have studied the existence and properties of the minimizers of the free energy by means of some rearrangements inequalities depending on the monotonicity assumption for the interaction potential U. As a matter of fact, the free energy is not jointly convex in the couple (ρ_1,ρ_2) at sufficiently low temperature, implying the non uniqueness of the minimizers and hence the phase transition. The general picture, at low temperature is the following: if the total masses of the two species are chosen in a appropriate interval, and the size of Ω is sufficiently large, compared to the range of the interaction, then, but for a small region, the densities take values close to the mean field densities $\rho^\pm$: $\rho_1=\rho^\pm$ and $\rho_2=\rho^\mp$.

The same question can be studied in the case $\Omega=\mathbb{R}$, with the conditions $\rho_1\to\rho^\pm$ and $\rho_2\to\rho^\mp$ as $x\to\pm\infty$. The solutions (called *fronts*) are studied in [4].

They are relevant in particular for the study of the interface between regions occupied by different phases. Indeed, in the so called *sharp interface* limit, they can be used as the lowest order approximation to the densities ρ_i across the interface region along the normal direction to the separating surface. This question has been discussed in [5], [6] where it is shown that the macroscopic equations governing the motion of the fluid are given by the incompressible Navier-Stokes equations for the continuous velocity field, with pressure having a jump on the separating surface, proportional to the curvature of the surface and to the free energy computed in terms of the microscopic interaction. The normal velocity of the separating surface on the other hand equals the normal component of the velocity field. This picture is obtained by bulk and interface matching expansions in the mean free path. The validity of the expansions is still open.

A very relevant question to be addressed in this context is the dynamical stability of the equilibrium solutions and its relation with the thermodynamic stability expressed by the minimizing property of the free energy. At the moment we have no answer for the model we have presented above, but we have better understanding for a related model where the thermalizing collisions are replaced by the interaction with a reservoir at temperature T modeled by a Fokker-Plank operator. This means that we replace the previous evolution equations with

$$\partial_t f_1 + v\cdot\nabla_x f_1 + F_1\cdot\nabla_v f_1 = Lf_1$$

$$\partial_t f_2 + v\cdot\nabla_x f_2 + F_2\cdot\nabla_v f_2 = Lf_2,$$

$$Lf(v) = \nabla_v\left(M_T\nabla\left(\frac{f}{M_T}\right)\right),\quad M_T(v)=\frac{\mathrm{e}^{-v^2/2T}}{(2\pi T)^{3/2}}.$$

The equilibrium solutions for this model are the same as those of the previous model and are the minimizers of the same free energy. In particular, one can study the stability of the fronts with respect to small initial perturbations. This problem has been faced in [7] by means of an energy method strongly relying on the free energy minimizing properties of the equilibrium. Indeed, they imply some spectral gap for the second Frechet derivative of the free energy, used as a partial norm measuring the size of the perturbation. The asymptotic stability of the front solution it then proved in L_2 both for the perturbation and its spatial and time derivatives. Assuming spatial decay of the initial perturbation, one can also show its algebraic decay in time.

In conclusion, the binary gas model presented here seems to be a good laboratory to test conjectures and mathematical techniques on the study of the dynamics of phase transitions. A few mathematical results have been obtained but many problems are still open.

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Stability of fronts in systems of conservation laws

H. Freistühler

Under certain assumptions, the evolution of fluids and solids including phase boundaries moving within them can be modeled by systems of conservation laws. The talk focuses on the sharp-interface case (no higher-order effects present in the PDE model) and on the question in which way and to which extend discontinuities in waves modeling phase boundaries can be treated analogously to shock waves. While shock waves are subsonic-supersonic and the Rankine-Hugoniot jump conditions (solely expressing the effects of conservation at the interface) suffice to determine the local dynamics, the typical subsonicity of phase boundaries rises a well-posedness problem, at first sight. Various proposals have been made to remedy the apparent deficiency by adding complementary boundary conditions at the

free interface, these extra conditions go under the name of "kinetic rules". The speaker's own results (obtained together with S. Benzoni-Gavage and R. Plaza, respectively) concern (a) liquid-vapor phase boundaries in a van-der-Walls like fluid, (b) martensite twins formed in elastic materials. Regarding (a) we have shown local-in-time persistence for the case of a new kinetic rule that explicitely incorporates surface tension as a singular measure on the front. Technically this is a non-standard normal modes analysis/construction of a Kreiss symmetrization. Regarding (b), again local-in-time persistence is shown to go hand in hand with certain requirements on the kinetic rule; the later are satisfied e.g. for the speed driving fraction rule proposed by Abeyaratne and Knowles.

On the variational approximation of second and fourth order geometric evolution equations

Harald Garcke
(joint work with John Barrett and Robert Nürnberg)

Many phase transition problems lead to situations in which an interface moves according to a velocity law involving the mean curvature. Typical examples are the mean curvature flow

$$\mathcal{V} = \kappa \tag{1}$$

and the surface diffusion flow

$$\mathcal{V} = -\Delta_s \kappa\,. \tag{2}$$

Here, Δ_s is the Laplace-Beltrami operator, $\mathcal{V}$ and κ are respectively the normal velocity and the mean curvature of a smooth evolving hypersurface in $\mathbb{R}^d$ which we denote by $\Gamma = (\Gamma_t)_{t\geq 0}$. For closed surfaces $(\Gamma_t)_{t\geq 0}$ it can be computed that the above flows are surface area decreasing and the surface diffusion flow in addition preserves the volume in cases where the evolving surface encloses a volume.

It was the goal of my presentation to introduce a novel finite element approximation of the above flows which can also handle generalizations including anisotropic situations and cases in which triple junctions appear. As suggested first by Dziuk [5] we use the identity

$$\Delta_s \vec{x} = \vec{\kappa} = \kappa \vec{\nu}$$

as a basis to introduce a finite element method for geometric evolution equations which involve the mean curvature. Above $\vec{x}$ is the parametrization of the surface, $\vec{\kappa}$ is the mean curvature vector and $\vec{\nu}$ is a unit normal to Γ_t. Let me in the following describe how the above identity can be used to solve the evolution equations

$$\mathcal{V} = f(\kappa) \quad \text{and} \quad \mathcal{V} = -\Delta_s \kappa \tag{3}$$

numerically. Here we assume that $f : (a, b) \to \mathbb{R}$ with $-\infty \leq a < b \leq \infty$ is a strictly monotonically increasing function. The choice $f(r) = -r^{-1}$ leads to the inverse mean curvature flow which has applications e.g. in general relativity.

For parametrizations $\vec{x} : \Omega \times [0,T] \to \mathbb{R}^d$ of Γ, where Ω is a suitable reference manifold without boundary in $\mathbb{R}^d$ we rewrite the equations in (3) as

$$\mathcal{V} := \vec{x}_t \cdot \vec{\nu} = f(\kappa) \ , \ \kappa\vec{\nu} = \Delta_s \vec{x} \tag{4}$$

and

$$\vec{x}_t \cdot \vec{\nu} = -\Delta_s \kappa \ , \ \kappa\vec{\nu} = \Delta_s \vec{x} \, , \tag{5}$$

respectively. The idea is to approximate the functions $\vec{x}$ and the mean curvature κ by piecewise linear continuous finite elements. This leads to an evolution problem for polyhedral surfaces which can be discretized in time by using a semi-implicit approach.

Let Γ^m be a *polyhedral surface* in $\mathbb{R}^3$ approximating the closed surface $\Gamma(t_m)$, $m = 0 \to M$. Following [5], we now parameterize the new closed surface Γ^{m+1} over Γ^m. Hence, given $\vec{X}^m$, a parameterization of Γ^m, we introduce the following finite element spaces. Let $\Gamma^m = \bigcup_{j=1}^J \overline{\sigma_j^m}$, where $\{\sigma_j^m\}_{j=1}^J$ is a family of mutually disjoint open triangles with vertices $\{\vec{q^m}_k\}_{k=1}^3$. Then for $m = 0 \to M-1$, let

$$\underline{V}(\Gamma^m) := \{\vec{\chi} \in C(\Gamma^m, \mathbb{R}^3) : \vec{\chi}|_{\sigma_j^m} \text{ is linear } \forall \ j = 1 \to J\} =: [W(\Gamma^m)]^3, \tag{6}$$

where $W(\Gamma^m) \subset H^1(\Gamma^m, \mathbb{R})$ is the space of scalar continuous piecewise linear functions on Γ^m, with $\{\phi_k^m\}_{k=1}^K$ denoting the standard basis of $W(\Gamma^m)$.

For scalar and vector functions $u, v \in L^2(\Gamma^m)$ we introduce the L^2 inner product $\langle \cdot, \cdot \rangle_m$ over the current polyhedral surface Γ^m, which is described by the vector function $\vec{X}^m$, as follows

$$\langle u, v \rangle_m := \int_{\Gamma^m} u \, . \, v \, \mathrm{d}s.$$

If u, v are piecewise continuous, with possible jumps across the edges of $\{\sigma_j^m\}_{j=1}^J$, we introduce the mass lumped inner product $\langle \cdot, \cdot \rangle_m^h$ as

$$\langle u, v \rangle_m^h := \tfrac{1}{3} \sum_{j=1}^J |\sigma_j^m| \sum_{k=0}^2 (u \, . \, v)((\vec{q}_{j_k}^m)^-), \tag{7}$$

where $\{\vec{q}_{j_k}^m\}_{k=0}^2$ are the vertices of σ_j^m, i.e. $\overline{\sigma_j^m} = \triangle\{\vec{q}_{j_k}^m\}_{k=0}^2$, and where we define $u((\vec{q}_{j_k}^m)^-) := \lim_{\sigma_j^m \ni \vec{p} \to \vec{q}_{j_k}^m} u(\vec{p})$. Here $|\sigma_j^m| = \frac{1}{2} \, |(\vec{q}_{j_1}^m - \vec{q}_{j_0}^m) \times (\vec{q}_{j_2}^m - \vec{q}_{j_0}^m)|$ is the measure of σ_j^m. In addition, we introduce the outward unit normal $\vec{\nu}^m$ to Γ^m; that is,

$$\vec{\nu}_j^m := \vec{\nu}^m \, |_{\sigma_j^m} := \frac{(\vec{q}_{j_1}^m - \vec{q}_{j_0}^m) \times (\vec{q}_{j_2}^m - \vec{q}_{j_0}^m)}{|(\vec{q}_{j_1}^m - \vec{q}_{j_0}^m) \times (\vec{q}_{j_2}^m - \vec{q}_{j_0}^m)|} \, , \tag{8}$$

where we have assumed that the vertices $\{\vec{q}_{j_k}^m\}_{k=0}^2$ are ordered anti-clockwise on the outer surface of σ_j^m. Finally, we set $|\cdot|_{m(,h)}^2 := \langle \cdot, \cdot \rangle_m^{(h)}$.

We propose the following approximation to (4) using a semi-implicit time discretization with time step $\tau > 0$: Given Γ^0 and the identity function $\vec{X}^0 \in \underline{V}(\Gamma^0)$

on Γ^0, then for $m = 0 \to M-1$ find $\{\vec{X}^{m+1}, \kappa^{m+1}\} \in \underline{V}(\Gamma^m) \times W(\Gamma^m)$ such that

$$\text{(9a)} \qquad \langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi\, \vec{\nu}^m \rangle_m^h - \langle f(\kappa^{m+1}), \chi \rangle_m^h = 0 \qquad \forall\ \chi \in W(\Gamma^m),$$

$$\text{(9b)} \qquad \langle \kappa^{m+1}\, \vec{\nu}^m, \vec{\eta} \rangle_m^h + \langle \nabla_s\, \vec{X}^{m+1}, \nabla_s\, \vec{\eta} \rangle_m = 0 \qquad \forall\ \vec{\eta} \in \underline{V}(\Gamma^m);$$

where, as noted above, the inner products $\langle \cdot, \cdot \rangle_m^{(h)}$ as well as ∇_s depend on m.

Moreover, we propose the following approximation to (5): Given Γ^0 and the identity function $\vec{X}^0 \in \underline{V}(\Gamma^0)$ on Γ^0, then for $m = 0 \to M-1$ find $\{\vec{X}^{m+1}, \kappa^{m+1}\} \in \underline{V}(\Gamma^m) \times W(\Gamma^m)$ such that

$$\text{(10a)} \qquad \langle \frac{\vec{X}^{m+1} - \vec{X}^m}{\tau_m}, \chi\, \vec{\nu}^m \rangle_m^h - \langle \nabla_s\, \kappa^{m+1}, \nabla_s\, \chi \rangle_m = 0 \qquad \forall\ \chi \in W(\Gamma^m),$$

$$\text{(10b)} \qquad \langle \kappa^{m+1}\, \vec{\nu}^m, \vec{\eta} \rangle_m^h + \langle \nabla_s\, \vec{X}^{m+1}, \nabla_s\, \vec{\eta} \rangle_m = 0 \qquad \forall\ \vec{\eta} \in \underline{V}(\Gamma^m).$$

For a different approach to approximate surface diffusion we refer to [1].

We can establish the following results for (9a), (9b) and (10a), (10b) respectively under very mild assumptions on the triangulations:

- There exists a unique solution to the discrete systems.
- The discretizations are stable and in particular surface area decreasing.
- A continuous in time, discrete in space variant of (10a), (10b) preserves the enclosed volume.
- The schemes have very good properties with respect to the distribution of mesh points. For curves and a fully implicit discretization this generically leads to equidistribution of mesh points. For surfaces the good mesh properties can be explained with the help of conformal mappings.
- Triple and multiple junctions and anisotropy can be included.

For details we refer to [2], [3], [4].

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Competition of Mutation and Selection in Multitype Branching Processes

Hans-Otto Georgii
(joint work with Ellen Baake)

We consider multitype branching processes in continuous time. Each individual x has a type $\sigma(x)$ belonging to a finite set S. It lives for an exponential time span with parameter $a_{\sigma(x)}$, after which it splits into a random number of offspring individuals of possibly different types; the offspring distribution depends on x only via its type $\sigma(x)$. Life spans and offspring numbers of different individuals are independent. Let $X(t)$ denote the set of all individuals living at time t, and $Z(t) = \sum_{x\in X(t)} \delta_{\sigma(x)}$ the measure on S that counts the individuals of each type at time t. That is, $Z_j(t)$ is the number of j-individuals in $X(t)$.

The basic information on the type evolution is captured in the generator $A = (a_i(m_{ij} - \delta_{ij}))_{i,j\in S}$; here, m_{ij} is the expected offspring of type j of an i-individual, and δ_{ij} is Kronecker's delta. Namely, if $\mathbb{E}^i$ denotes the expectation for the process starting with a single i-individual, then $\mathbb{E}^i(Z_j(t)) = (e^{tA})_{ij}$ for all $i, j \in S$. We assume throughout that A is irreducible. The Perron-Frobenius theorem then implies that

$$\mathbb{E}^i(Z_j(t))\, e^{-\lambda t} \underset{t\to\infty}{\longrightarrow} h_i\, \pi_j\,,$$

where λ is the principal eigenvalue of A, π a left eigenvector, and h a right eigenvector of λ, both of which are positive and normalised by $\langle \pi, 1\rangle = 1 = \langle \pi, h\rangle$. This means that λ is the mean growth rate, h_i the long-term fertility of type i, and π the type distribution of the population in the infinite future. It will turn out that a further distribution of interest is $\alpha = (\pi_i\, h_i)_{i\in S}$, which plays a role as ancestral type distribution; see below.

In the following, we confine ourselves to the supercritical case $\lambda > 0$, in which the population survives forever with positive probability. The role of π and α is then elucidated by the following two almost-sure convergence results. On the one hand,

$$Z(t)/|X(t)| \underset{t\to\infty}{\longrightarrow} \pi \quad \mathbb{P}^i\text{-almost surely conditioned on survival.}$$

This means that π is the almost-sure equilibrium type distribution of the population when one looks forward from an ancestor into the future, and is part of the classical Kesten-Stigum theorem; see [4] for the continuous-time version of the simple argument in [5]. On the other hand, for an individual $x \in X(t)$ let $x(s)$ be its ancestor at time $s < t$, and $L^x(t) = \frac{1}{t}\int_0^t \delta_{\sigma(x(s))}\, ds$ the empirical type distribution along the whole ancestral line. Then

$$\frac{1}{|X(t)|} \sum_{x\in X(t)} \delta_{L^x(t)} \underset{t\to\infty}{\longrightarrow} \delta_\alpha \quad \mathbb{P}^i\text{-almost surely conditioned on survival.}$$

That is, α is the type distribution that emerges by looking from a typical individual $x \in X(t)$ backwards into its past; this was proved in [4].

To specify the behaviour of the process in more detail, we now split the generator A into its mutational part $u_{ij} = a_i\,(m_{ij} - m_i\ \delta_{ij})$ (where $m_i = \sum_{i\in S} m_{ij}$ is the expected total offspring of an i-individual), and the reproduction part $r_i = a_i\,(m_i - 1)$. That is, A is the sum of the Markov generator $U = (u_{ij})$ and the diagonal matrix with entries r_i. Using a size-biased tree construction analogous to but different from that in [5], one then finds $\mathbb{E}^i(|X(t)|) = \widetilde{\mathbb{E}}^i(e^{t\langle L^\xi(t),r\rangle})$, where $\xi(t)$ is a continuous-time Markov chain with generator U that describes the mutations along a particular random lineage. By Varadhan's lemma of large deviation theory, it thus follows that

$$\lambda := \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}^i(|X(t)|) = \max_\nu [\langle \nu, r\rangle - I_U(\nu)]\,,$$

where the maximum extends over all probability measures ν on S, and I_U is the rate function associated with $\xi(t)$. This variational principle describes the competition of mutation and reproduction that determines the growth rate λ. The maximum on the right is attained precisely for α. That is, α shows the right balance of mutation and reproduction that is needed for maximal growth.

In the paper [2], we try to understand this competition in more detail. We fix a type characteristic $\varrho : S \to \mathbb{R}$ and consider the constrained growth rate

$$\begin{aligned}\Lambda(z) &= \lim_{\varepsilon\to 0} \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}^i\Big(\sum_{x\in X(t)} 1_{\{|\langle L^x(t),\varrho\rangle - z|\le\varepsilon\}}\Big) \\ &= \max_{\nu:\ \langle\nu,\varrho\rangle = z} [\langle \nu, r\rangle - I_U(\nu)]\end{aligned}$$

that describes the growth rate of the subpopulation with average lineage characteristic $z \in \mathbb{R}$. By partial convex conjugation, $\Lambda(z)$ can be expressed in terms of the total growth rates for populations with the same mutation matrix U but reproduction rates of the form $r + \beta\varrho$ with varying β.

We analyse $\Lambda(z)$ in the particular case of sequence space models. For simplicity, we consider here only the binary case and let $S = \{0,1\}^N$. The natural type characteristics is then $\varrho : \omega \mapsto \frac{1}{N}\sum_{k=1}^N \omega_k$, which can be interpreted as the average deviation from a wildtype. We assume that the mutation and reproduction rates depend only on $\varrho(\omega)$, so that we can project our branching process onto the simpler type space $S = \{0, \frac{1}{N}, \ldots, 1\}$. We assume further that U is reversible. This gives us an eplicit expression for the rate function I_U, and allows us to pass to the process with the *symmetric* mutation generator $F_{ij} = \sqrt{U_{ij}U_{ji}}$ for $i \neq j$, and reproduction rates $E_i := r_i + \sum_{j\in S} \sqrt{U_{ij}U_{ji}}$. The latter process has the same λ and $\Lambda(z)$. So we can use the results of [1], which present a Laplace approximation for λ in the limit $N \to \infty$, when the F_{ij} and E_i allow for a smooth approximation in this limit. This leads us to the following result: *If $E_i = e(i) + O(1/N)$ for some $e \in C^2[0,1]$ and the F_{ij} satisfy a similar approximation condition then*

$$\Lambda(z) = \hat{e}(z) + O(N^{-1/3}) \qquad \text{as } N \to \infty$$

locally uniformly in $z \in]0,1[$, where $\hat{e}$ is the concave envelope of e.

The fact that the concave envelope shows up here is an indication that a phase transition might occur. We checked this for the so-called quasispecies model of M. Eigen [3], in which a sequence $\omega \in \{0,1\}^N$ creates an offspring with rate $b(\varrho(\omega))$ and dies with rate $d(\varrho(\omega))$. On the occasion of birth, each site of the offspring sequence mutates from 0 to 1 with probability μ/N, and vice versa with probability ν/N. The symmetrised rates on the projected type space $S = \{0, \frac{1}{N}, \ldots, 1\}$ then allow for a natural but subtle Poisson approximation, and the above approximation of $\Lambda(z)$ holds with $e(z) := b(z)e^{-g(z)} - d(z)$, where $g(z) := (\sqrt{\mu(1-z)} - \sqrt{\nu z})^2$. The penalisation factor $e^{-g(z)}$ describes the loss of fitness outside a mutationally balanced region.

For a particular choice of the parameters, the above function e is non-concave. This means that all z with $e(z) < \hat{e}(z)$ do not contribute to the fitness of the population, and are suppressed during evolution in favour of those subpopulations for which $e(z) = \hat{e}(z)$. In particular, for a proper tuning of the reproduction rates, the function Λ attains its maximum at two different values of z, which means that the associated ancestral type distribution α has two distinct peaks. So one can speak of a "coexistence of phases" . A full understanding of these phenomena still requires further study.

As a final remark, let me mention that my cooperation with Ellen Baake started in Oberwolfach, where we met in 2000 for the first time.

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Entanglement entropy in the quantum Ising model

Geoffrey Grimmett

The object of this talk is to explain the relationship (formulated by Aizenman, Klein, and Newman in [1]) between the quantum Ising model and a classical model of probability theory termed the continuum random-cluster model, and to indicate how this may be exploited to obtain an estimate for the entanglement of a one-dimensional spin chain, in the strong-field regime. This work is joint with Tobias Osborne and Petra Scudo.

The state space of the quantum Ising model on a finite graph $G = (V, E)$ is the tensor product $\mathcal{H} = \bigotimes_{x \in V} \mathbb{C}^2$. As basis for the copy of $\mathbb{C}^2$ labelled by x, we take

the two eigenstates $|+\rangle_x$, $|-\rangle_x$ of the Pauli operator $\sigma_x^{(3)}$ at x, with corresponding eigenvalues ± 1. The other two Pauli operators are denoted $\sigma^{(1)}$ and $\sigma^{(2)}$. Let D be the set of $2^{|V|}$ basis vectors $|\eta\rangle$ for $\mathcal{H}$ of the form $|\eta\rangle = \bigotimes_x |\pm\rangle_x$, noting that D is in one–one correspondence with the space $\Sigma = \prod_{x\in V}\{-1,+1\}$.

The Hamiltonian of the quantum Ising model with transverse field is

$$H = -\tfrac{1}{2}\lambda \sum_{e=\langle x,y\rangle\in E} \sigma_x^{(3)}\sigma_y^{(3)} - \delta \sum_{x\in V} \sigma_x^{(1)}, \tag{1}$$

generating the operator $e^{-\beta H}$ where β denotes inverse temperature. Here, $\lambda, \delta \geq 0$ are the spin-coupling and transverse-field intensities, respectively. Let

$$\rho_G(\beta) = \frac{1}{\mathrm{tr}(e^{-\beta H})} e^{-\beta H}. \tag{2}$$

It is well known (see [1]) that the matrix elements of $\rho_G(\beta)$ may be expressed as a type of 'path integral' with respect to the continuum random-cluster model on $G \times [0,\beta]$ with parameters λ, δ and $q = 2$. Let $\Lambda = V \times [0,\beta]$, write Ω_Λ for the configuration space of the latter model, and let $\phi_{G,\beta}$ be the appropriate continuum random-cluster measure on Ω_Λ (with free boundary conditions). For $\omega \in \Omega_\Lambda$, let S_ω denote the space of all functions $s : V \times [0,\beta] \to \{-1,+1\}$ that are constant on the clusters of ω, and let S be the union of the S_ω over $\omega \in \Omega_\Lambda$. Given ω, we may pick an element of S_ω uniformly at random, denoted σ. For $s \in S$ and $W \subseteq V$, we write s_0 (respectively, s_β) for the vector $(s(x,0) : x \in V)$ (respectively, $(s(x,\beta) : x \in V)$).

Theorem 3. [1] The elements of the density matrix $\rho_G(\beta)$ satisfy

$$\langle \eta' | \rho_G(\beta) | \eta \rangle = \frac{\phi_{G,\beta}(\sigma_0 = \eta,\, \sigma_\beta = \eta')}{\phi_{G,\beta}(\sigma_0 = \sigma_\beta)}, \qquad \eta, \eta' \in \Sigma. \tag{4}$$

This representation may be used to study entanglement in the quantum Ising model on G. Let $W \subseteq V$, and consider the *reduced density matrix*

$$\rho_G^W(\beta) = \mathrm{tr}_{V\setminus W}(\rho_G(\beta)). \tag{5}$$

As above, the matrix elements may be expressed as the ratio of probabilities given in terms of a continuum random-cluster measure with a certain periodic boundary condition.

The *entanglement* of the vertex-set W relative to its complement $V \setminus W$ is interpreted here as the entropy $S_G^W = -\mathrm{tr}(\rho_G^W \log_2 \rho_G^W)$ where $\rho_G^W = \lim_{\beta\to\infty} \rho_G^W(\beta)$.

We specialise to the one-dimensional case. Let $m, L \geq 0$ and take $V = [-m, m+L]$ and $W = [0, L]$, viewed as subsets of $\mathbb{Z}$. We write $\rho_m(\beta)$ for $\rho_G(\beta)$, and S_m^L for S_G^W. A key step in the study of S_m^L for large m is a bound on the supremum norm of the difference $\rho_m^L - \rho_n^L$.

Theorem 6. [2] Let $\lambda, \delta \in (0,\infty)$ and write $\theta = \lambda/\delta$. There exist constants C, α, γ depending on θ and satisfying $\gamma > 0$ when $\theta < 1$ such that:

$$\|\rho_m^L - \rho_n^L\| \leq \min\bigl\{2, CL^\alpha e^{-\gamma m}\bigr\}, \qquad 2 \leq m \leq n < \infty. \tag{7}$$

One would expect that γ may be taken to satisfy $\gamma > 0$ under the weaker assumption $\lambda/\delta < 2$, but this has not yet been proved.

Theorem 8. [2] Let $\lambda, \delta \in (0, \infty)$ and write $\theta = \lambda/\delta$. There exists $\theta_0 \in (0, \infty)$ such that: for $\theta < \theta_0$, there exists $K = K(\theta) < \infty$ such that

$$S_m^L \leq K \log_2 L, \qquad m \geq 0,\ L \geq 2. \tag{9}$$

The two key properties of the continuum random-cluster model used in the proof are exponential decay of connectivities and the so-called ratio weak-mixing property.

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Stochastic approach to the quantum Curie-Weiss model

Dmitry Ioffe

(joint work with Marek Biskup, Lincoln Chayes, Nicholas Crawford, Anna Levit)

Classical Curie-Weiss mean-field Hamiltonian $\mathbf{H}_N^{\mathsf{CW}}$ is a function on $\Omega_N = \{\pm 1\}^N$,

$$-\mathbf{H}_N^{\mathsf{CW}}(\nu) \,=\, \frac{1}{N} \sum_{(i,j)} \nu_i \nu_j, \tag{1}$$

where the summation is over all unordered pairs of $i \neq j$. The values of the classical Hamiltonian $\left\{\mathbf{H}_N^{\mathsf{CW}}(\nu)\right\}$ could be viewed as eigenvalues of the quantum Hamiltonian $\mathcal{H}_N^{\mathsf{CW}}$,

$$\mathcal{H}_N^{\mathsf{CW}} \Psi_\nu \,=\, \mathbf{H}_N^{\mathsf{CW}}(\nu) \Psi_\nu, \quad \text{where} \quad -\mathcal{H}_N^{\mathsf{CW}} = \frac{1}{N} \sum_{(i,j)} \hat{\sigma}_i^{\mathsf{z}} \hat{\sigma}_j^{\mathsf{z}},$$

where $\hat{\sigma}^{\mathsf{z}}$ is the Pauli matrix

$$\hat{\sigma}^{\mathsf{z}} \,=\, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Given $\nu \in \{\pm 1\}^N$ he corresponding eigenvector $\Psi_\nu$equals to

$$\Psi_\nu \,\stackrel{\Delta}{=}\, \otimes_{i \in \Lambda} \psi_{\nu_i},$$

and,

$$\psi_{+1} \,=\, \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \text{and} \qquad \psi_{-1} \,=\, \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Accordingly, for a given value of the inverse temperature β, the distribution of ν is,

$$\mu_N^\beta(\nu) \;=\; \frac{1}{\mathcal{Z}_N}\mathrm{e}^{-\beta \mathbf{H}_N^{\mathsf{CW}}(\nu)} \;=\; \frac{\left\langle \Psi_\nu | \mathrm{e}^{-\beta \mathcal{H}_N^{\mathsf{CW}}(\nu)} | \Psi_\nu \right\rangle}{\mathsf{Tr}\left(\mathrm{e}^{-\beta \mathcal{H}_N^{\mathsf{CW}}(\nu)}\right)}. \tag{2}$$

One way to pin down phase transition in the CW model is to study statistical properties of the mean magnetization

$$\bar{\nu}_N \;\triangleq\; \frac{1}{N}\sum_i \nu_i,$$

under μ_N^β: The probability measure ν_N^β in (2) could be described in the following way: Let $\mathbb{Q}$ be the uniform $(1/2)$ distribution on $\{\pm 1\}$ and let $\otimes\mathbb{Q}$ be the corresponding product measure on $\Omega_N = \{\pm 1\}^N$. Then,

$$\mu_N^\beta(\nu) \;=\; \frac{\otimes\mathbb{Q}\left(\mathrm{e}^{N\beta(\bar{\nu}_N)^2/2}; \nu\right)}{\otimes\mathbb{Q}\left(\mathrm{e}^{N\beta(\bar{\nu}_N)^2/2}\right)}. \tag{3}$$

Then, elementary one-dimensional theory of large deviations implies that μ_N^β exponentially concentrates around

$$\left\{\nu \,:\, \bar{\nu}_N \text{ is close to } \operatorname{argmax}\left(\frac{\beta}{2}m^2 - I(m)\right)\right\},$$

where I is the large deviation rate function for $\bar{\nu}_N$ under $\otimes\mathbb{Q}$,

$$I(m) \;=\; \sup_h \left\{hm - \Lambda(h)\right\} \quad \text{and} \quad \Lambda(h) = \log \mathbb{Q}\left(\mathrm{e}^{h\nu}\right) = \log \frac{\mathrm{e}^h + \mathrm{e}^{-h}}{2}.$$

It is easy to see that I is strictly convex and differentiable on $(-1,1)$ with $I'(m) \to \pm\infty$ as $m \to \pm 1$. In particular, the supremum of $\beta m^2/2 - I(m)$ is actually attained inside $(-1,1)$ for any $\beta \in \mathbb{R}_+$. Furthermore, since $I(\cdot)/\beta$ is the convex conjugate of $\Lambda(\beta\cdot)/\beta$,

$$\operatorname{argmax}\left\{\frac{m^2}{2} - \frac{1}{\beta}I(m)\right\} \;=\; \operatorname{argmax}\left\{\frac{1}{\beta}\Lambda(\beta h) - \frac{h^2}{2}\right\}. \tag{4}$$

But $\Lambda(\beta\cdot)$ is the log-moment generating function of the $\pm\beta$ Bernoulli random variable. If we use $\mathbb{Q}_\beta$ for the corresponding distribution, then it is straightforward to check that the maximizers in (4) are of the form $\pm m^*(\beta)$, where $m^*(\beta) > 0$ iff,

$$\frac{1}{\beta}\mathbb{V}\mathrm{ar}_\beta(\nu) \;=\; \frac{\beta^2}{\beta}, \tag{5}$$

is larger than one. We, thereby, recover the critical value $\beta = 1$ of the classical CW model.

The main objective of this lecture is to explain that a very similar story happens with the quantum CW model in transverse field,

$$-\mathcal{H}_N^{\mathsf{CW}} \;=\; \frac{1}{N}\sum_{(i,j)}\hat{\sigma}_i^{\mathsf{z}}\hat{\sigma}_j^{\mathsf{z}} \;+\; \lambda\sum_i \hat{\sigma}_i^{\mathsf{x}}, \tag{6}$$

where $\lambda \geq 0$ is the strength of the transverse field and,

$$\hat{\sigma}^{\mathsf{x}} \;=\; \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

We associate with quantum Hamiltonian $\mathcal{H}_N^{\mathsf{CW}}$ in (6) classical probabilities,

$$\mu_N^{\beta,\lambda}(\nu) \;=\; \frac{\left\langle \Psi_\nu | \mathrm{e}^{-\beta\mathcal{H}_N^{\mathsf{CW}}(\nu)} | \Psi_\nu \right\rangle}{\mathsf{Tr}\left(\mathrm{e}^{-\beta\mathcal{H}_N^{\mathsf{CW}}(\nu)}\right)}. \tag{7}$$

Let $\mathrm{Prob}\lambda\beta$ be the distribution of the Poisson point process (of holes) on the circle $\mathbb{S}_\beta$ with arrival intensity λ. We shall use $\otimes\mathrm{Prob}\lambda\beta$ for the product distribution of N independent copies $\xi = (\xi_1, \ldots, \xi_N)$. For every i let $\#(\xi_i)$ be the number of connected components of $\mathbb{S}_\beta \setminus \xi_i$. Evidently, the number of all compatible $\nu \sim \xi$ equals to $2^{\sum_i \#(\xi_i)}$. Define

$$\widetilde{\mathbb{P}}_\beta^\lambda(\mathrm{d}\xi) \;=\; \frac{2^{\#(\xi)}\mathrm{Prob}\lambda\beta(\mathrm{d}\xi)}{\mathrm{Prob}\lambda\beta\left(2^{\#(\xi)}\right)}$$

Consider probability distribution $\mathbb{Q}_\beta^\lambda$ on piece-wise constant classical one-circle spin trajectories $\nu : \mathbb{S}_\beta \mapsto \{\pm 1\}$ which is generated by the following two step procedure: First sample ξ from $\widetilde{\mathbb{P}}_\beta^\lambda$, and then paint connected components of $\mathbb{S}_\beta \setminus \xi$ into ± 1, independently and with probability $1/2$ each. Let $\otimes\mathbb{Q}_\beta^\lambda$ be the corresponding product measure. The path integral approach to (7) reveals that an analysis of phase diagram of the CW model in transverse filed boils down to an investigation of asymptotic properties for weighted (path) measures

$$\otimes\widetilde{\mathbb{Q}}_\beta^\lambda(\mathrm{d}\nu) \;\triangleq\; \frac{\otimes\mathbb{Q}_\beta^\lambda\left(\exp\left\{\frac{N}{2}\int_0^\beta \left(\bar{\nu}_N(t)\right)^2 \mathrm{d}t\right\}\,;\,\mathrm{d}\nu\right)}{\otimes\mathbb{Q}_\beta^\lambda\left(\exp\left\{\frac{N}{2}\int_0^\beta \left(\bar{\nu}_N(t)\right)^2 \mathrm{d}t\right\}\right)}, \tag{8}$$

where,

$$\bar{\nu}_N(t) \;=\; \frac{1}{N}\sum_i \nu_i(t).$$

This problem belongs to the realm of theory of large deviations. Formally, the measures (8) are asymptotically concentrated around solutions of

$$\sup_m\left\{\frac{1}{2}\int_0^\beta m^2(t)\mathrm{d}t \;-\; I(m)\right\} \;\triangleq\; \sup_m \mathfrak{G}(m), \tag{9}$$

where I is the large deviation rate function for the average $\bar{\nu}_N$ under the product measures $\otimes\mathbb{Q}_\beta^\lambda$. If we formulate the large deviation principle in $\mathbb{L}_2(\mathbb{S}_\beta)$, then, using

$(\cdot,\cdot)_\beta$ for the corresponding scalar product,

$$I(m) \;=\; \sup_h \{(h,m)_\beta - \Lambda(h)\} \quad \text{where} \quad \Lambda(h) \;=\; \log \mathbb{Q}_\beta^\lambda \left(\mathrm{e}^{(h,\nu)_\beta}\right). \tag{10}$$

It happens that the critical curve is implicitly given by

$$\mathfrak{f}(\lambda,\beta) \;\stackrel{\Delta}{=}\; \frac{1}{\beta}\mathbb{V}\mathrm{ar}_\beta^\lambda\left((\nu,\mathbf{1})_\beta\right) \;=\; \frac{1}{\lambda}\tanh(\lambda\beta) \;=\; 1, \tag{11}$$

where $\mathbb{V}\mathrm{ar}_\beta^\lambda$ is the variance under the one-circle spin measure $\mathbb{Q}_\beta^\lambda$. In fact, the variational problem (9) has constant maximizers $\pm m^*(\lambda,\beta)\mathbf{1}$, where the spontaneous z-magnetization m^* satisfies:

(1) If $\mathfrak{f}(\lambda,\beta) \le 1$, then $m^* = 0$.
(2) If $\mathfrak{f}(\lambda,\beta) > 1$, then $m^* > 0$, and, consequently there are two distinct solutions to (9).

Furthermore, away from the critical curve the solutions $\pm m^*\mathbf{1}$ are stable in the following sense: There exists $c = c(\lambda,\beta) > 0$ and a strictly convex symmetric function U with $U(0) = 0$ and $U''(0) > 0$, such that

$$\mathfrak{G}(\pm m^*\mathbf{1}) - \mathfrak{G}(m) \;\ge\; c\min\left\{\|m - m^*\mathbf{1}\|_\beta^2, \|m + m^*\mathbf{1}\|_\beta^2\right\} + \int_0^\beta U(m'(t))\mathrm{d}t. \tag{12}$$

Phase Transitions in Aperiodic Crystals

Ted Janssen

Phase transitions with a change of symmetry from a high-symmetry group G_0 to a low-symmetry group H may be described in the framework of the Landau theory. This describes the free energy as a polynomial in an order parameter η. The first terms are

$$F \;=\; \frac{a(T)}{2}\eta^2 + \frac{1}{4}\eta^4.$$

The order parameter belongs to an irreducible representation of the group G_0. The new symmetry group then is the subgroup for which the elements are represented by the unit matrix.

For crystals the symmetry groups are usually the space groups G_0 and H. The order parameter belongs to an irreducible representation which is characterised by a star of wave vectors k and a representation of the 'little group' G_k which is the group of elements which leave k invariant.

However, there are many materials showing a phase transition from a structure with three-dimensional space group symmetry to an aperiodic structure, where the latter has equally perfect long range order as the other phase. These materials have sharp diffraction peaks at positions of a Z-module, called the Fourier module. The wave vectors are of the form

$$\mathbf{k} \;=\; \sum_{i=1}^n h_i \mathbf{a}_i^*,$$

where n is larger than the space dimension, and where h_i are integers. The number of rationally independent vectors (n) is the rank of the Fourier module. These materials do not have three-dimensional space group symmetry. Usually the Euclidean symmetry is rather low. The transition from periodic to aperiodic structure can still be described using Landau theory, because the new phase belongs to a representation of the original space group[1, 2]. However, for further transitions between phases one has to use another technique in order to be able to use Landau theory.

The vectors $\mathbf{k}$ are considered as projections of reciprocal lattice vectors $\mathbf{k}_s$ in an abstract n-dimensional space: $\mathbf{k} = \pi\mathbf{k}_s$. Furthermore, the aperiodic structure, having a density function $\rho(\mathbf{r})$, is embedded in this n-dimensional 'superspace' by

$$\rho_s(\mathbf{r}, \mathbf{r}_I) \;=\; \sum_{\mathbf{k}_s} \rho(\pi\mathbf{k}_s) \exp(i\mathbf{k}.\mathbf{r} + i\mathbf{k}_I.\mathbf{r}_I).$$

Because of the construction the n-dimensional density ρ_s is lattice periodic, and consequently has n-dimensional space group theory.

Phase transitions from or to such an aperiodic crystal state can now be described using Landau theory. One has to distinguish two cases. In the first place the rank of the structures on both sides of the phase transition can be equal. In that case the groups G_0 and H are both n-dimensional space groups. The free energy is a function of the order parameter, which corresponds to a representation of the space group. In the case that the ranks are not equal one has to embed the space of the lower rank system into a space of the higher rank structure. For example, for the transition from a three-dimensional space group symmetric structure to an aperiodic crystal of rank n, the transition is described in an n-dimensional space. The original symmetry group is then the product $G_0 \times E^d$ of the three-dimensional space group and the Euclidean group in $d = n - 3$ dimensions. The irreducible representations of this group are easily constructed. The superspace group after the transformation is the subgroup of elements represented by the unit operator.

This procedure has been applied to several examples of the four main classes of aperiodic crystal structures: incommensurate modulated structures, incommensurate composites, quasicrystals and incommensurate magnetic structures. In all the classes examples of transitions between phases with equal or with unequal rank have been found. For quasicrystals, for example, these are transitions from aperiodic to an approximant (1st order) and the transtion from quasicrystal to modulated quasicrystal, where the rank changes from 6 to 12. For composites there are subsystems showing a change in the unit cell resulting in a different Fourier module of the same rank, and models showing an increase in the rank at the phase transition[4]. The symmetries occurring in magnetic phase transitions may be described in Landau theory using representations of groups, superspace groups and magnetic symmetry groups with operators combining space transformations and time reversal[3].

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Nucleation and growth for the Ising model in dimension three or higher

Francesco Manzo

(joint work with R. Cerf)

The talk concerns the metastable relaxation of the kinetic Ising model (Metropolis dynamics) in the regime of infinite volume and vanishing temperature. It is a joint work with R. Cerf.

We extend the two dimensional result of Dehghanpour and Schonmann to an arbitrary dimension.

The formal energy function associated with a configuration $\eta \in \{-1,+1\}^{\mathbb{Z}^d}$ is

$$E^d(\eta) := -\frac{1}{2} \sum_{\substack{x,y\in\mathbb{Z}^d \\ \|x-y\|=1}} \eta(x)\eta(y) - \frac{h}{2} \sum_{x\in\mathbb{Z}^d} \eta(x). \tag{1}$$

Let $-\mathbf{1}$ (resp. $\mathbf{1}$) denote the configuration with spin minus in every site of the $d-$dimensional lattice $\mathbb{Z}^d$. We consider a small positive 'magnetic' field h, so that the minimizer of the energy is $\mathbf{1}$.

We prove that for sufficiently small positive magnetic field h, for each $\epsilon > 0$ there exists $\mathrm{d} > 0$ such that for sufficiently large inverse temperature β and every local observable f,

$$\mathbb{E}(f(\sigma_t^d)) = f(-\mathbf{1}) + o(e^{-\beta \mathrm{d}}) \quad \text{for any } t < e^{\beta(\kappa_d - \epsilon)} \tag{2}$$

$$\mathbb{E}(f(\sigma_t^d)) = f(\mathbf{1}) + o(e^{-\beta \mathrm{d}}) \quad \text{for any } t > e^{\beta(\kappa_d + \epsilon)}, \tag{3}$$

σ_t^d denotes the $d-$dimensional kinetic Ising model starting from $-\mathbf{1}$ and where the constant κ_d is related to the $i-$dimensional 'communication hights' Γ_i by

$$\kappa_d = \frac{1}{d+1} \sum_{i=1}^{d} \Gamma_i. \tag{4}$$

In the regime we are considering, the relaxation pattern is characterized by the formation of suitable 'critical droplets' ('nucleation') and by their growth.

We follow the strategy developed by Dehghanpour and Schonmann for the two-dimensional case, using inductive ideas to relate the behavior of the $d-$dimensional process with the $(d-1)$-dimensional one.

As regards nucleation, we show that the formation rate is the same as in the finite-volume case.

In order to get this result, and use the well-developed finite-volume techniques, we need a bound on the probability that te process in a given point is influenced by far-away spins.

Unlike in the two-dimensional case, we are unable to characterize geometrically the metastable cycle and in particular we do not know the inner details of the 'metastable cycle' that could help a droplet of pluses to cross a long distance. Instead, we use the ferromagnetic properties of the energy giving a quite general description of the cycle structure for attractive systems.

Once the nucleation problem is reconducted to the finite-volume case, we have to rule out the possibility that the process is trapped in some deep well. Again, our knowledge of the energy landscape is insufficient in order to follow the standard strategies.

We take advantage of the attractivity of the dynamics to get uniform bounds for the nucleation probability within time $\exp(-\beta(\kappa_d \pm \epsilon))$.

The main difficulty concerns the estimate of the speed of growth of a super-critical droplet. Heuristically, we can imagine that a big cube of pluses grows via the formation of a $(d-1)$-dimensional critical droplet that grows with the $(d-1)$-dimensional speed. This idea is at the basis of our inductive scheme.

For combinatorial reasons (and complex geometrical problems), we are not able to use the 'chronological path' argument used by Dehghanpour and Schonmann. Instead, we abandon large deviation techniques and set up a construction that gives super-exponential bounds on the probability that the droplet grows by $\exp(\beta\epsilon)$ within time $\exp(\beta(\kappa_{d-1} - \epsilon))$.

This construction can be applyed in other contexts like boostrap percolation.

Displacement convexity and minimal fronts at phase boundaries

Rossana Marra

(joint work with E. A. Carlen, M. C. Carvalho, R. Esposito, J.L. Lebowitz)

We consider minimization problems for a type of functional that arises in the study of phase segregation in statistical mechanical systems. Let $F(m)$ be a function on the real line that is continuous and strictly positive except at $m = a$ and $m = b$ with $a < b$.

Let $\mathcal{C}_{a,b}$ be the set of functions $m(x)$ from $\mathbb{R}$ to $\mathbb{R}$ such that

$$\lim_{x\to-\infty} m(x) = a \qquad \text{and} \qquad \lim_{x\to+\infty} m(x) = b \ .$$

The numbers a and b represent the values of the order parameter m in two phases of a statistical mechanical system. For example, $m = a$ might correspond to a vapor phase, and $m = b$ to a liquid phase.

Then a function $m(x)$ in $\mathcal{C}_{a,b}$ denotes a possible *transition profile* across the boundary segregating the two different phases. The actual profile that one would

expect to see would be one that minimizes the free energy cost of making such a transition. Here, the free energy functional $\mathcal{F}$ to be minimized on $\mathcal{C}_{a,b}$ is

$$\mathcal{F}(m) = \int_{\mathbb{R}} F(m(x))\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} (m(x)-m(y))^2 J(x-y)\mathrm{d}x\mathrm{d}y \ ,$$

where $J(x)$ is a non-negative integrable function on $\mathbb{R}$.

The term $\int_{\mathbb{R}} F(m(x))\mathrm{d}x$ is due to short range interactions and entropy effects, while the term $\int_{\mathbb{R}}\int_{\mathbb{R}}(m(x)-m(y))^2 J(x-y)\mathrm{d}x\mathrm{d}y$ is due to long range interactions. This long range term in the free energy suppresses sharp transitions.

Much useful information can be deduced from the specific form of the minimizing profiles. In particular, the surface tension at a phase boundary is the minimum value of $\mathcal{F}(m)$ on $\mathcal{C}_{a,b}$. Hence we ask:

• *What is the minimum value of $\mathcal{F}(m)$ as m ranges over $\mathcal{C}_{a,b}$, and the minimizing profiles, if any, unique up to translation?*

Note that the existence of minimizers is relatively simple. Because of the translation invariance, they are never unique: Any translate of a minimizer is again a minimizer. It is less simple to show that this is the only degeneracy.

Displacement convexity and uniqueness of fronts.

For a particular choice of F in the free energy functional $\mathcal{F}$, this problem has been solved in a series of papers [6],[7] by DeMasi, Orlandi, Triolo and Presutti. Their solution involves the construction of a dynamics that is dissipative for the free energy functional, and then a careful analysis of limits along the time evolution for this dynamics.

Another approach that we further develop here has been introduced by Alberti and Bellettini [2], [1]. They discovered an alternative convex structure which renders the variational problem for $\mathcal{F}$ convex, and used this to study the existence problem in [2]. Later, Alberti returned to the problem proving in [1] a uniqueness result that affirmatively answers the question raised above for this one component model.

Our goal here is to treat certain two component systems. Motivated by this problem, we were led to reconsider the single component problem from the point of view of McCann's notion of *displacement convexity* [8].

In fact, the minimization problem for $\mathcal{F}$ is challenging largely because the functional $\mathcal{F}$ is *not convex* on $\mathcal{C}_{a,b}$ in the usual way: For $0 < \lambda < 1$, and m_0 and m_1 in $\mathcal{C}_{a,b}$, define $m_\lambda = (1-\lambda)m_0 + \lambda m_1$ and note that $m_\lambda \in \mathcal{C}_{a,b}$. However, due to the non convexity of the potential function F, it is *not* true in general that $\mathcal{F}(m_\lambda) \leq (1-\lambda)\mathcal{F}(m_0) + \lambda\mathcal{F}(m_0)$.

There is however, another convex structure with respect to which $\mathcal{F}$ *is* convex. This convex structure cannot be defined on all of $\mathcal{C}_{a,b}$, but only on the subset of *monotone* profiles $\mathcal{M}_{a,b}$. Nothing is lost in this restriction, as a rearrangement inequality of Alberti [1] shows that minimizers of $\mathcal{F}$ on $\mathcal{C}_{a,b}$ must actually lie in

$\mathcal{M}_{a,b}$. Any profile $m(x)$ increasing monotonically from a to b can be written as

$$m(x) = a + (b-a)\int_{-\infty}^{x} \mathrm{d}\mu(y)$$

where μ is a probability measure on $\mathbb{R}$. This identification of $\mathcal{M}_{a,b}$ and the set of probability measures on $\mathbb{R}$ allows us to look at $\mathcal{F}$ as a functional defined on probability measures.

On the set of probability measures on $\mathbb{R}$ (or more general domains) there is an alternative convex structure that was introduced by McCann [8], building on groundbreaking work of Brenier [3]. It is based on a measurable map $T : \mathbb{R} \to \mathbb{R}$, which is used to define a notion of transport of a measure μ_0 into another measure μ_1: $\mu_1 = T\#\mu_0$, *push forward of* μ_0 *under* T. A functional on probability measures is said to be *displacement convex* if it is convex with respect to this alternative structure. We show that $\mathcal{F}$, regarded as a functional on probability measures is in fact displacement convex, and also strictly convex, namely $\frac{d^2}{d\lambda^2}\mathcal{F} > 0$ and is equal to zero unless the map T is a translation. This implies the uniqueness of the minimizer up to translations. It is easy to show that the local part of the functional, $F(m)$, is affine, since this new notion of convexity naturally look at $F(m)$ as a function on the inverse function $x(m)$ [2]. To show that the non local part is convex we introduce a potential $W(x-y)$ whose second derivative is related to $J(x-y)$ and use the positivity of J to show the convexity of W.

This solution to the variational problem has the advantage of applying also for free energy functionals in certain multicomponent systems, introduced in [4] and [5], describing a binary fluid, in which the determination of the minimizers has not been previously treated.

Binary fluid functional.

The system is made of two different species of particles and the particle number densities are denoted by $m(x)$ and $n(x)$. The functional $\mathcal{G}$ defined by

$$\mathcal{G}(m,n) = \int_{\mathbb{R}} \left[m(x)\ln m(x) + n(x)\ln n(x) + \beta \int_{\mathbb{R}} \bar{J}(x-y)m(x)n(y)\mathrm{d}y - g_{\beta,\mu} \right] \mathrm{d}x$$

is the *excess free energy* at a front. Here, $g_{\beta,\mu} = \inf_{m,n\geq 0} f_{\beta,\mu,\mu}(m,n)$ and

$$f_{\beta,\mu_1,\mu_2}(m,n) = m\ln m + n\ln n + \beta\hat{J}mn - \mu_1 m - \mu_2 n$$

is the thermodynamic free energy. The functional has made of two part: the entropy and the energy associate to a repulsive interaction between the two species. The functional is not convex at low temperature, due to the presence of a phase segregation transition with coexistence of two phases, one richer in one species and the other richer in the second species. We look for the minimizers of this functional for $\beta > \beta_c$, which represents the phase boundary. The minimum value gives the surface tension across the phase boundary.

We prove that this functional is displacement convex on the set $\mathcal{M}_{\rho^-,\rho^+} \times \mathcal{M}_{\rho^+,\rho^-}$ of the monotone profiles with fixed asymptotic values $\rho^{\pm}$ at infinity. We

prove also that it is strictly displacement convex up to translations. As a consequence, we get the following theorem.

Theorem
If (w_1, w_2) and (v_1, v_2) are any two critical points of $\mathcal{G}$ in $\mathcal{M}_{\rho^-,\rho^+} \times \mathcal{M}_{\rho^+,\rho^-}$, then there is an $a \in R$ so that

$$(v_1(x), v_2(x)) = (w_1(x-a), w_2(x-a)) \ .$$

Thus, there is exactly one critical point (w_1, w_2) such that $w_1(0) = w_2(0)$. It is symmetric in the sense that $w_1(x) = w_2(-x)$ for all x.

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Magnetic domain wall motion

Christof Melcher

(joint work with Antonio Capella and Felix Otto)

We investigate the gyrotropic motion of a magnetic domain wall in a (soft) magnetic thin film with an applied field $H = H(t)$ pointing along the easy axis. Our analysis is based on the following Landau-Lifshitz-Gilbert equation

$$\partial_t \mathbf{m} + \alpha\, \mathbf{m} \wedge \partial_t \mathbf{m} + \varepsilon\, \gamma\, \mathbf{m} \wedge \nabla E(\mathbf{m}) = \varepsilon\, \gamma\, H(t)\, \big(\mathbf{m} \wedge \mathbf{e_2}\big)$$

for parameterized transition layers that are periodic

$$\mathbf{m}(t) : \mathbb{R} \times \mathbb{T} \to \mathbb{S}^2 \quad \text{with} \quad \mathbf{m}(\pm\infty, t) = (0, \pm 1, 0)$$

where $\nabla E_\varepsilon(\mathbf{m})$ is the L^2 gradient of the reduced domain wall energy

$$E_\varepsilon\big(\mathbf{m}\big) = \frac{1}{2} \int_{\mathbb{R}\times\mathbb{T}} \left(\mathcal{Q}\, |\nabla \mathbf{m}|^2 + (1 - m_2^2) + \Big(\frac{m_3}{\varepsilon}\Big)^2 \right)\, dx + \frac{1}{2} \int_{\mathbb{R}\times\mathbb{T}\times\mathbb{R}} |\nabla u|^2\, dx$$

$$\text{where} \quad \Delta u = \operatorname{div}\, \big(\mathbf{m}\, \delta_{\{x_3=0\}}\big) \quad \text{distributionally on } \mathbb{R} \times \mathbb{T} \times \mathbb{R}.$$

The parameter $\varepsilon \ll 1$ corresponds to the relative thickness (i.e. thickness/exchange length) and triggers the effect of anisotropy. We are interested in the singular limit as $\varepsilon \to 0$, that is the evolution equation for a Néel wall. For this purpose we consider a sequence of solutions $\mathbf{m}^\varepsilon$ of LLG with uniformly bounded initial energy.

Theorem 1. *Suppose that* $\alpha(\varepsilon)/\varepsilon \to \nu$ *and* $\mathbf{m}^\varepsilon \rightharpoonup \mathbf{m}$ *weakly in* $L^2_{\mathrm{loc}}(\mathbb{R}\times\mathbb{T}\times(0,T))$. *Then* $\mathbf{m} = (m, 0)$ *where* $m(t) : \mathbb{R}^2 \to \mathbb{S}^1$ *is a weak solution of*

$$\Big[\partial_t^2 m + \nu\,\partial_t m + \nabla E_0(m)\Big] \cdot m^\perp = 0$$

where

$$E_0(m) = \frac{1}{2}\int_{\mathbb{R}\times\mathbb{T}} \big(\mathcal{Q}\,|\nabla m|^2 + m_1^2\big)\; dx + \frac{1}{2}\int_{\mathbb{R}\times\mathbb{T}\times\mathbb{R}} |\nabla u|^2\; dx.$$

Observe that the limiting equation is a geometric wave equations. A related singular limit for LLG but with fixed damping coefficient α has first been found by E and Garcia [3]. In their result the gyromagnetic term becomes effectively a damping term whereas in our result oscillatory features are potentially preserved. Of particular interest is the case of flat Néel walls, where the stray-field interaction reduces to the $H^{1/2}$ self-interaction of the first component function. The corresponding variational principle can conveniently expressed as

$$\begin{aligned} E_0(m) = \frac{1}{2}\Big(\mathcal{Q}\,\|m\|^2_{\dot H^1} + \|m_1\|^2_{\dot H^{1/2}} + \|m_1\|^2_{L^2}\Big) &\to \min \\ \text{for} \quad m : \mathbb{R} \to \mathbb{S}^1 \quad \text{with} \quad m(\pm\infty) &= (0, \pm 1). \end{aligned}$$

The problem of a static Néel wall, including its internal two-scale structure, logarithmic energy decay, and typical extremely slow logarithmic decay behavior of Néel wall profiles, has been analyzed, see [6, 7, 2]. In a dynamic context we aim for a description in terms of a mechanical analog

$$M\,\ddot q + \frac{1}{\beta}\,\dot q = H(t)$$

where $q = q(t)$ is the wall center, at least for small forcing $H = H(t)$. The construction of dynamic solutions near by the static Néel requires stability. It can be shown that Néel walls indeed strict minimizers modulo translations. Introducing a phase θ so that $m = (\cos\theta, \sin\theta)$ the reduced LLG dynamics of a Néel wall reads

$$\partial_t^2\theta + \nu\,\partial_t\theta + \nabla\mathcal{E}(\theta) = H(t)\,\cos\theta$$

where $\mathcal{E}(\theta) = E_0(m)$ is the Néel wall energy. We have the following results:

Theorem 2. *For sufficiently small constant field strength* H *there exists a traveling wave for the reduced Landau-Lifshitz-Gilbert dynamics*

$$c^2\,\theta'' + c\,\nu\,\theta' + \nabla\mathcal{E}(\theta) = H\cos\theta$$

that connects antipodal states at infinity $\theta(\pm\infty) = \pm\pi/2$ *near the static Néel wall* θ_0. *Moreover, the propagation speed has an expansion*

$$c = \beta H + o(H)$$

where the wall mobility is given by $\beta = 1/(M\nu)$ *with* $M = \frac{1}{2}\int |\theta_0'|^2\; dx$.

Theorem 3. *There exists $\eta > 0$ so that whenever $T \geq 1$ and H is T-periodic with*

$$\int_0^T |H(t)|^2 dt + T^2 \int_0^T |\dot{H}(t)|^2 \, dt < \eta^2$$

then there is an T-periodic solution $\theta = \theta(x,t)$ for the reduced LLG

$$\partial_t^2 \theta + \nu \, \partial_t \theta + \nabla \mathcal{E}(\theta) = H(t) \cos \theta$$

that connects antipodal states at infinity and so that

$$\theta(x,t) = \theta_0(x + q(t)) + \psi(x,t)$$

where $\|\psi\| = \mathcal{O}(\eta)$ and the wall center $q = q(t)$ satisfies

$$M \, \ddot{q} + M \, \nu \, \dot{q} = H(t) + o(\eta).$$

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Interface profile for 1 d ferromagnetic Ising model with long range interaction

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(joint work with Marzio Cassandro, Utikir Rozikov)

It is well known that a one dimensional Ising spin system with ferromagnetic long range interactions which decay as $|x-y|^{-2+\alpha}, \alpha \in [0, \frac{1}{2}]$ exhibits a phase transition [1],[2].

To study the phase coexistence region we consider a finite volume $2L+1$ with mixed boundary conditions ($-$ on the left and $+$ on the right) and use a geometrical description for the spin configurations σ, introduced in a previous paper [3] that allows to describe the energy fluctuations as a gas of interacting contours. This representation is similar to that already introduced by [2] but more transparent and easier to handle. We define a "phase-separating" point and we study its

statistical properties. (i.e. the magnetization profile where, say, the boundary conditions are negative on the left and positive on the right).

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Γ-convergence for rate-independent processes with applications to damage

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(joint work with G. Bouchitté and T. Roubíček)

1. Introduction

We consider an elastic body $\Omega \subset \mathbb{R}^d$ and want to describe the damage evolution under given Dirichlet boundary conditions in the part $\Gamma_{\rm Dir}$ of the boundary $\partial\Omega$. In particular, we are interested in the situation that the damage can be complete, i.e., the material can disintegrate (e.g., into powder) such that the displacement $u : \Omega \to \mathbb{R}^d$ is no longer defined.

We denote by $\mathbf{e}(u) = \frac{1}{2}(\nabla u + \nabla u^{\mathsf{T}})$ the infinitesimal strain tensor and by $z : \Omega \to [0,1]$ a scale damage variable with $z = 1$ in the case of no damage and $z = 0$ if everything breakable is broken. The stored-energy functional is given in the form

$$\widehat{\mathcal{E}}(u,z) = \int_\Omega W(x,\mathbf{e}(u)(x),z(x)) + \frac{\kappa}{r}|\nabla z(x)|^r \mathrm{d}x, \tag{1}$$

where $W(x,\mathbf{e},\cdot)$ decreases with respect to $z \in [0,1]$, since damage weakens the material. The case of incomplete damage is mathematically described by uniform coercivity (in $z \in [0,1]$), whereas in the case of complete damage we usually assume only

$$\textbf{nonuniform coercivity:} \quad W(x,\mathbf{e},z) \geq cz|\mathbf{e}|^p - C, \tag{2}$$

i.e., coercivity in $\mathbf{e}$ is present as long as the damage is not yet complete.

Loss of coercivity leads to problems in defining the displacement, even when $W(x,\cdot,z)$ is convex. We assume that elasticity is always in equilibrium, i.e., $u(t)$ should be the minimizer of $\mathcal{E}(\cdot,z(t))$ on $\mathrm{W}^{1,p}(\Omega;\mathbb{R}^d)$ under the condition $u|_{\Gamma_{\rm D}} = U_{\rm D}(t)$. However, missing coercivity will lead to nonattainment of the minimum due to location in the regions of total damage. Nevertheless, it is of practical interest in civil engineering to model the further development of damage in other parts of the body where damage is not yet complete.

We suggest to treat the problem by looking at energy densities and stress distributions instead of the displacements or the strains. Under the simple assumption $|\partial_{\mathbf{e}} W(x,\mathbf{e},z)| \le C W(x,\mathbf{e},z)$ it is easy to see that bounded energies lead to bounded stresses in $\mathrm{L}^1(\Omega)$. In particular, we show that introducing a small damage threshold $\delta > 0$, we obtain solutions (u_δ, z_δ), and it is possible to show that for a subsequence we have $z_\delta(t) \to z(t)$, where z solves an appropriate limit problem in terms of an energy functional obtained as Γ-limit. Moreover, the energies, stresses and the power of the time-dependent boundary conditions converge to the limit values.

2. Model for incomplete damage

The model with incomplete damage was studied in [MR06], and we recall the main ingredients here.

For $p \in]1,\infty[$ assume that the time-dependent boundary conditions satisfy $u_D \in \mathrm{C}^1([0,T];\mathrm{W}^{1,p}(\Omega;\mathbb{R}^d))$. The stored-energy density $W : \Omega \times \mathbf{E}_d \times [0,1] \to \mathbb{R}$ is Caratheodory, convex in $\mathbf{e}$ and satisfies the uniform coercivity $\forall \mathbf{e}, z\colon c|\mathbf{e}|^p - C \le W(\mathbf{e},z) \le C|\mathbf{e}|^p + C$ as well as the uniform stress control

$$\forall \mathbf{e}, z\colon |\partial_{\mathbf{e}} W(\mathbf{e},z)| \le C W(\mathbf{e},z). \tag{3}$$

For the regularizing term in (1) we assume $r > d$.

The stored-energy potential is given as $\mathcal{E}(t,u,z) = \widehat{\mathcal{E}}(u + u_{\mathrm{Dir}}(t), z)$ and the dissipation distance as $\mathcal{D}(z_0,z_1) = \begin{cases} \int_\Omega \rho(z_0 - z_1)\mathrm{d}x & \text{if } z_1 \le z_0, \\ \infty & \text{else.} \end{cases}$ Both are defined on the state space $\mathcal{Q} = \mathcal{F} \times \mathcal{Z}$ with $\mathcal{F} = \{\, u \in \mathrm{W}^{1,p}(\Omega;\mathbb{R}^d) \mid u|_{\Gamma_{\mathrm{D}}} = 0 \,\}$ and $\mathcal{Z} = \{\, z \in \mathrm{W}^{1,r}(\Omega) \mid z \in [0,1] \text{ a.e. in } \Omega \,\} \Subset \mathrm{C}^0(\overline{\Omega})$.

Theorem 5 ([MR06])**.** *For all $q_0 \in \mathcal{S}(0)$ there exists an energetic solution $q = (u,z) : [0,T] \to \mathcal{Q}$ with $q(0) = q_0$, i.e., for all $t \in [0,T]$ the global stability (S) and the energy balance (E) hold:*

(S) $\forall\, \mathrm{wt}\, q = (\mathrm{wt}\, u, \mathrm{wt}\, z) \in \mathcal{Q}\colon \mathcal{E}(t,q(t)) \le \mathcal{E}(t,\mathrm{wt}\, q) + \mathcal{D}(z(t),\mathrm{wt}\, z)$

(E) $\mathcal{E}(t,q(t)) + \mathrm{Diss}_{\mathcal{D}}(z,[0,t]) = \mathcal{E}(0,q(0)) + \int_0^t \partial_\tau \mathcal{E}(\tau,q(\tau))\mathrm{d}\tau.$

Moreover, we have $u \in \mathrm{L}^\infty([0,T];\mathrm{W}^{1,p}(\Omega;\mathbb{R}^d))$ and $z \in \mathrm{L}^\infty([0,T];\mathrm{W}^{1,r}(\Omega)) \cap \mathrm{BV}([0,T];\mathrm{L}^1(\Omega))$.

The proof is based on time-incremental minimization problems and used the abstract methods developed in [MM05, DFT05, Mie05].

3. Complete damage

We eliminate the displacement u by minimization with respect to u. However, this only works properly as long as we have some coercivity. We assume now only the nonuniform coercivity (2) and assume further that $W(\cdot,z)$ is convex on $\mathbf{E}_d = \mathbb{R}^{d\times d}_{\mathrm{sym}}$ and still satisfies the uniform stress control (3). We define the

functionals $\mathcal{E}_\delta(t,u,z) = \mathcal{E}(t,u,z+\delta)$ and $\mathcal{I}_\delta(t,z) = \min_{u\in\mathcal{F}} \mathcal{E}(t,u,z+\delta)$. Using the strain space $\mathrm{L}^p(\Omega,\mathbf{E}_d)$ with $\mathbf{E}_d = \mathbb{R}^{d\times d}_{\mathrm{sym}}$ we define $\mathcal{H}_\delta : \mathrm{L}^p(\Omega,\mathbf{E}_d)\times\mathcal{Z}\to\mathbb{R}$ via

$$\mathcal{H}_\delta(\widehat{\mathbf{e}},z) = \mathcal{G}_\delta(\widehat{\mathbf{e}},z) + \int_\Omega \frac{\kappa}{r}|\nabla z|^r \mathrm{d}x \quad \text{with } \mathcal{G}_\delta(\widehat{\mathbf{e}},z) = \min_{u\in\mathcal{F}} \int_\Omega W(\widehat{\mathbf{e}}+\mathbf{e}(u),z+\delta)\mathrm{d}x.$$

Clearly, we have $\mathcal{I}_\delta(t,z) = \mathcal{H}_\delta(\mathbf{e}_{\mathrm{D}}(t),z)$ and $\partial_t\mathcal{I}_\delta(t,z) = \langle \mathrm{D}_{\mathbf{e}}\mathcal{G}_\delta(\mathbf{e}_{\mathrm{D}}(t),z), \dot{\mathbf{e}}_{\mathrm{D}}(t)\rangle$, where $\mathbf{e}_{\mathrm{D}} = \mathbf{e}(u_{\mathrm{Dir}})$. Note that $\sigma = \mathrm{D}_{\mathbf{e}}\mathcal{H}_\delta(\mathbf{e},z) = \mathrm{D}_{\mathbf{e}}\mathcal{G}_\delta(\mathbf{e},z) \in \mathrm{L}^{p'}(\Omega;\mathbf{E}_d)$ defines an equilibrium stress.

The previous section allows us to construct solutions q_δ associated with $(\mathcal{E}_\delta,\mathcal{D})$. The limit $\delta\to 0$ is obtained using the abstract Γ-convergence for rate-independent processes developed in [MRS07]. Using the monotonicity in δ the Γ-limits

$$\mathbb{I}(t,\cdot) = \Gamma\text{-}\lim_{\delta\to 0} \mathcal{I}_\delta(t,\cdot), \quad \mathbb{G}(\widehat{\mathbf{e}},\cdot) = \Gamma\text{-}\lim_{\delta\to 0} \mathcal{G}_\delta(\mathbf{e},\cdot).$$

The following universal way of calculating the Γ-limit is very useful:

$$\mathbb{G}(\mathbf{e},z) = \lim_{\epsilon\searrow 0}\Big(\lim_{\delta\searrow 0} \mathcal{G}_\delta(\mathbf{e},(z-\epsilon)^+)\Big).$$

As a consequence we find that $\mathbb{G}(\cdot,z) : \mathrm{L}^p(\Omega;\mathbf{E}_d)\to[0,\infty[$ is convex and that $\mathbb{I}(t,z) = \mathbb{G}(\mathbf{e}_{\mathrm{D}}(t),z) + \int_\Omega \frac{\kappa}{r}|\nabla z|^r \mathrm{d}x$. For quadratic $W(\cdot,z)$, i.e.

$$W(\mathbf{e},z) = \frac{1}{2}\mathbf{e}{:}\mathbb{C}(z){:}\mathbf{e},$$

it can then be shown that $\mathbb{I}(\cdot,z)\in\mathrm{C}^1([0,T])$ and

$$z_\delta \rightharpoonup z \text{ and } \mathcal{I}_\delta(t,z_\delta)\to\mathbb{I}(t,z) \quad\Longrightarrow\quad \partial_t\mathcal{I}_\delta(t,z_\delta)\to\partial_t\mathbb{I}(t,z).$$

Thus, all the assumption of the abstract theory in [MRS07] are satisfied and the following result is established.

Theorem 6 ([BMR07])**.** *Under the above assumptions (including the restrictive assumption that W is quadratic) the energetic limit problem associated with $(\mathbb{I},\mathcal{D})$ has for each stable initial condition a solutions.*

Moreover, if $z_\delta{:}[0,T]\to\mathcal{Z}$ are energetic solutions associated with $(\mathcal{I}_\delta,\mathcal{D})$ and the initial data satisfy $z_\delta(0)\rightharpoonup z^0$ and $\mathcal{I}_\delta(0,z_\delta(0))\to\mathcal{I}(0,z^0)$, then there exists a subsequence $(z_{\delta_k})_{k\in\mathbb{N}}$ and $\mathrm{wt}\, z : [0,T]\to\mathcal{Z}$ such that $\mathrm{wt}\, z$ is an energetic solution for $(\mathcal{I},\mathcal{D})$ with $\mathrm{wt}\, z(0) = z^0$ and for all $t\in[0,T]$ we have

(1) $z_{\delta_k}(t)\to\mathrm{wt}\, z(t)$ *in* $\mathrm{W}^{1,r}(\Omega)$ *(strong!),*

(2) $\mathcal{I}_\delta(t,z_{\delta_k}(t))\to\mathbb{I}(t,\mathrm{wt}\, z(t))$, $\mathrm{Diss}_{\mathcal{D}}(z_{\delta_k},[0,t])\to\mathrm{Diss}_{\mathcal{D}}(\mathrm{wt}\, z,[0,t])$,

(3) $\sigma_k(t) = \mathrm{D}_{\mathbf{e}}\mathcal{G}_{\delta_k}(\mathbf{e}_{_D}(t),z_{\delta_k}(t))\rightharpoonup \mathrm{wt}\,\sigma(t) = \mathrm{D}_{\mathbf{e}}\mathbb{G}(\mathbf{e}_{_D}(t),\mathrm{wt}\, z(t))$ *in* $\mathrm{L}^2(\Omega;\mathbf{E}_d)$,

(4) $\partial_t\mathcal{I}_\delta(t,z_\delta)\to\partial_t\mathbb{I}(t,z)$.

It remains open to generalize the above result to more general densities W allowing for nonquadratic cases and to reducing the exponent r to $1\le r\le d$.

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Traffic jams, symmetry breaking and ordering far from thermal equilibrium

David Mukamel

It is well known that phenomena like breaking of ergodicity, spontaneous symmetry breaking and condensation do not take place in one dimensional systems in thermal equilibrium. This is true provided the system is at finite temperature and the interaction between particles is short range.

In the present talk we consider the steady state of driven systems. It is demonstrated that these steady states can exhibit phase transitions, ergodicity breaking and spontaneous symmetry breaking when the dynamics is local and noisy. This is done by a detailed analysis of specific models of driven one dimensional systems.

A simple model of a driven system in one dimension, introduced some time ago, is the ABC model [1, 2]. This is a lattice model where each lattice point is occupied by one of three types of particles, A, B or C. The model evolves under local dynamical rules, whereby a randomly chosen pair of nearest neighbor particles are exchanges with some rates which do not obey detailed balance. The dynamics is local and conserves the three densities. A simple argument suggesting that the model should phase separate and break the translational symmetry is given. It is also shown that for the special case where the three densities are equal the steady state distribution is governed by an effective Hamiltonian with long range interactions. This provides a simple mechanism for breaking of ergodicity in one dimension. Here, although the dynamics is local, the resulting effective Hamiltonian is long ranged which makes symmetry breaking possible.

Following this demonstration, a criterion for the existence of phase separation in driven density conserving one dimensional systems is discussed [3]. It is suggested that phase separation is related to the size dependence of the steady-state currents of domains in the system. A quantitative criterion for the existence of phase separation is conjectured using a correspondence made between driven diffusive

models and zero-range processes. Several driven diffusive models are discussed in light of the conjecture.

A class of models of driven diffusive systems which is shown to exhibit phase separation in one dimension is introduced [4]. Unlike all previously studied models exhibiting similar phenomena, here the phase separated state is fluctuating in the bulk of the macroscopic domains. The nature of the phase transition from the homogeneous to the phase separated state is discussed in view of a criterion introduced above for phase separation in one-dimensional driven systems.

The question of existence of phase separation in one dimensional systems is closely related that that of traffic jams. Thus the studies discussed above have been used to consider the jamming phenomena. It is suggested that the question of existence of a jamming phase transition in a broad class of single-lane cellular-automaton traffic models may be studied using a correspondence to the asymmetric chipping model [5]. In models where such correspondence is applicable, jamming phase transition does not take place. Rather, the system exhibits a smooth crossover between free-flow and jammed states, as the car density is increased.

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Hydrodynamics of a disordered lattice gas with random reservoir.

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(joint work with Mustapha Mourragui)

We consider a lattice gas interacting by the exclusion rule in the presence of a quenched random field given by i.i.d. bounded random variables in a bounded domain in contact with random reservoirs. We show that the rescaled density field almost sure, with respect to the random field, converges to the unique weak solution of a d- dimensional parabolic equation with boundary conditions. This type of problem is motivated by the recent developments on the non-equilibrium processes based on the analysis of stationary measures and large deviations properties.

In the last years there has been several papers devoted in understanding macroscopic properties of non equilibrium systems. Typical examples are systems in contact with two thermostats at different temperature or with two reservoirs at different densities, see [1] and references there in. In this paper we focus on the first step, namely on the derivation of macroscopic limit (hydrodynamic limit) for a particles system evolving according to local- conservative dynamics (Kawasaki)

with hard core exclusion rule and with rates depending on a quenched random field in a cylinder domain $d \geq 3$ in which the basis, denoted Γ are kept at different densities. The rates are chosen so that the system satisfies a detailed balance condition with respect to a family of random Bernoulli measures (the random field Ising model at infinite temperature). To model the presence of the reservoirs as in previous papers one superimposes on the boundary to the local-conservative dynamics a jump dynamics (creation and destruction of particle). The rates which we considered depend on the quenched random field as well and are chosen so that the random Bernoulli measure with a suitable choice of the chemical potential is reversible for the dynamics of birth and death process. This latter dynamic is of course not conservative and keeps the fixed value of the density on Γ. There is a flow of density through the full system and the full dynamic is not reversible. Such systems have been used to model electron transport in doped crystals. In this case the exclusion rule is given by the Pauli principle and the presence of impurities in the crystals is the origin of the presence of quenched random field, see [5]. The presence of the random field together with the exclusion rule makes the problem high not trivial. The transport properties of such systems in the case of periodic boundary condition on Γ has been studied by Faggionato and Martinelli [2]. They derived in $d \geq 3$, the hydrodynamic limit and a variational formula for the bulk diffusion $D(\cdot)$, which is equivalent to the Green-Kubo formula. They proved that the bulk diffusion depends on the statistical properties of the quenched random field but not on the randomness itself. So far there are no results in such direction for dimension $d = 1$ and $d = 2$. Dynamical large deviations for the same model and always with periodic boundary conditions have been derived in [7] as special case of a more general system discussed there. The bulk dynamics turns out to be of the so-called *nongradient* type. Roughly speaking, the gradient condition says that the microscopic current is already the gradient of a function of the density field. Further it is not translation invariant, for a given disorder configuration. To model the interaction with the reservoirs we superimpose at the boundary a birth and death process in which the rates depend still by the quenched random field. In order to prove the hydrodynamic behavior of the system, we follow the entropy method introduced by Guo, Papanicolau and Varadhan [3]. It relies on an estimate of the entropy of the states of process with respect to a reference invariant state. The main problem is that in the model considered the reference invariant state is not explicitly known. To overcome this difficulty we compute the entropy of the state of the process with respect to a product measure with slowly varying profile. Obviously, since this measure is not invariant, the entropy does not need to decrease and then we need to estimate the rate at which it increases. This type of strategy has been used in previous papers dealing with the same type of problems, see [4] and [6], which considered generalized exclusion process of non gradient type. The main difference with the mentioned papers is the presence of the randomness in the model we are considering. This forces to take random birth and death rates. Then, we need to apply an ergodic theorem to obtain the final

result. The equation we obtain for the local particles density is the following:

$$
(1) \qquad \begin{aligned} \partial_t \rho &= \nabla \cdot \Big(D(\rho) \nabla \rho \Big) , \\ \rho(0, \cdot) &= \rho_0 , \\ \rho(t, \cdot)\big|_\Gamma &= b(\cdot) \quad \text{for} \quad t > 0 , \end{aligned}
$$

where $b(\cdot) \in (0,1)$ is a smooth function and $\rho_0 \in L^\infty[\Lambda; (0,1)]$ is the initial profile.

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Avalanches in first-order phase transitions

Antoni Planes

(joint work with Erell Bonnot, Eduard Vives, and Lluís Mañosa)

Many different materials undergoing a first-order phase transition need to be driven by an external field (intensive parameter) for the transition to occur. Thus, the transition extends over a certain range of the driving field and usually takes place through a sequence of discontinuous steps or avalanches of the order parameter. These avalanches reflect the fact that the system relaxes from a (marginally stable) metastable state towards another metastable state with an associated energy dissipation (responsible for the hysteresis observed in these transitions). Typically, the metastable minima are separated by very high energy barriers and, therefore, the transition kinetics is not dominated by thermal fluctuations (athermal behaviour). The configuration of metastable minima determines a complex free-energy landscape which is at the origin of the properties of these systems: the noisy nature of response to the driving field and mesoscale phase separation reflected in a polyvariant structure [1]. Martensitic materials are typical examples of this class of systems. In these materials avalanches are related to sudden changes in the local strain field. These changes give rise to acoustic emission (AE) waves in the range

from kHz to MHz which can be detected by means of adequate transducers [2]. The study of these transient acoustic waves is of great interest since they provide relevant information related to the relaxation kinetics from one metastable state to another. It is worth noting that the AE in martensitic (elastic) systems is the analog of Barkhausen noise in magnetic materials, which is associated with sudden changes of the local magnetization. Furthermore, the phenomenology is typical of a broad class of systems characterized by a complex free-energy landscape with many metastable local minima, a consequence of the existence of disorder and also of long-range (anisotropic) interactions which are operative during the transition. In addition to magnetic and elastic systems, other examples where similar phenomenology has been reported include ferroelectric [3] and superconductor [4] systems. The existence of long-range interactions is the essential ingredient to understand the formation of the polyvariant structures observed in these materials. In elastic systems, the physical cause of these interactions is the coherency strain between the parent and martensitic phases, which can be conveniently expressed by taking into account the long range coupling between the strain tensor components resulting from elastic compatibility constraints [5]. Disorder is important for the nucleation of the product phase and thus in determining the specific path followed by the system at the transformation.

An interesting feature regarding AE is the power-law behaviour of the distribution of amplitudes and duration of the emitted acoustic signals. This reveals a lack of characteristic scales related to size and duration of the avalanches and therefore to some kind of criticality. This criticality can be understood within the framework of lattice models with (different kinds of) quenched disorder following athermal (T = 0 K) dynamics corresponding to local energy relaxation [6]. Due to this local character, the evolution of the system when driven by an external field will not, in general, follow an equilibrium path, but rather evolve through metastable states. By numerical simulations one obtains hysteresis loops consisting of a sequence of avalanches. The corresponding avalanche size (and duration) distribution changes from supercritical to subcritical by increasing the amount of disorder. Interestingly, criticality is found for a given amount of disorder which suggests the existence of disorder induced criticality. In magnetic systems this has been confirmed from scaling analysis of hysteresis loops in systems with controlled amounts of disorder [7]. In martensitic transitions this has been checked by taking advantage of the fact that dislocations are formed during the transformation process. Therefore, the amount of disorder can be modified by cycling through the transition. Thus, starting with a virgin sample (suitably heat treated), it has been shown that the distribution of the amplitudes of the acoustic signals (avalanches) evolves from supercritical to critical with the number of cycles [8]. This feature is expected to be a consequence of a combined effect of the amount and distribution of disorder and of the long-range interactions that determine the suitable free-energy landscape to enable criticality.

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Translation invariance of Gibbsian point processes in two dimensions

Thomas Richthammer

Gibbs measures or Gibbsian point processes serve as a model for equilibrium states of interacting particle systems in statistical physics. (For an introduction to the lattice version of this model we refer to the book of H.-O. Georgii [3].) Here a particle is described by a point in $\mathbb{R}^d \times S$, where d is the number of spatial dimensions and S is a set describing internal properties of the particle. The interaction is given in terms of a two-body potential U and a chemical potential $-\log z$, where the so called activity parameter $z > 0$ can be thought of regulating the particle density. In general it is a difficult problem to find all equilibrium states for a particle system with given interaction U and activity z, and often one has to be satisfied with finding out interesting properties of the set of all equilibrium states. An important example for such a property is the conservation of a symmetry: A symmetry g is defined to be a transformation on the particle space such that U is g-invariant. The symmetry is said to be conserved if all equilibrium states are g-invariant, otherwise it is said to be broken. As the breaking of a symmetry forces the system to exhibit a phase transition, there is a strong motivation to investigate these properties. Our aim is to find conditions on U and z which imply the conservation of a given symmetry g of U. We will restrict ourselves to the case of the symmetry of spatial translations. Here the most interesting case is the one of $d = 2$ spatial dimensions. The first results in this case were obtained by J. Fröhlich and C.-E. Pfister ([1],[2]), their arguments relying on the smoothness of the potential U. In [5] and [6] we showed how the conservation of translational

symmetry can also be shown for discontinuous and hard core potentials. In this extended abstract we will focus on describing how to deal with hard cores and for clarity we will restrict ourselves to the simplest interaction with a hard core, namely pure hard core repulsion or the hard sphere model.

In the hard sphere model the interaction takes the simple form

$$U_{hc}(x_1, x_2) := \begin{cases} \infty & \text{for} \quad |x_1 - x_2| \leq r \\ 0 & \text{for} \quad |x_1 - x_2| > r, \end{cases}$$

where $x_1, x_2 \in \mathbb{R}^2$, $|.|$ is a norm on $\mathbb{R}^2$ and $r > 0$. Having a Boltzmann factor in mind, the form of U implies that any two particles are forced to keep a distance $> r$ from one another (hard core condition). Thus here a particle can be considered to be a sphere of radius $r/2$ such that any two of these spheres are forbidden to overlap. We note that U_{hc} is translation invariant. In spite of the simple form of U_{hc} not much is known about this model, see the article of H. Löwen [4]. Our result is the following:

Theorem 7. *For any activity $z > 0$ all equilibrium states corresponding to U_{hc} and z are translation invariant, i.e. in the two-dimensional hard sphere model the translational symmetry is conserved.*

In the following we consider a translation in a fixed direction $\vec{e} \in \mathbb{R}^2$ by a fixed translation distance $\tau \in \mathbb{R}$. The main idea of the the proof in the smooth case is to replace this constant translation by a position dependent translation transformation $x \mapsto x + \tau_n(x)\vec{e}$, where $\tau_n = \tau$ in some neighbourhood of the origin, $\tau_n = 0$ far away (at distance n) from the origin and such that τ_n is a suitably chosen interpolation for positions in between. In the hard core case however, this kind of independent transformation does not work, because here the transformation has to respect the hard core property: Every configuration of particles satisfying the hard core condition has to be transformed in such a way that after the transformation the condition still holds. Thus the transformation of a certain particle affects the transformation of all particles in its neighbourhood. The most important tool in the proof of Theorem 1 is thus a transformation $\mathfrak{T}_n$ on the set of all particle configurations such that in the construction of $\mathfrak{T}_n(X)$ for a configuration X every particle $x \in X$ is translated a certain distance $t_{n,X}(x)$ in direction $\vec{e}$ and we have the following properties:

(1) Every particle x near the origin is translated the distance τ.
(2) Every particle x far from the origin (at distance n) is translated by 0.
(3) $\mathfrak{T}_n$ respects the hard core.
(4) $\mathfrak{T}_n$ is bijective and the transformation of the Poisson point process by $\mathfrak{T}_n$ admits a density φ_n.
(5) We have a suitable estimate on this density.

However, it turns out that these properties are conflicting: E.g. properties (1),(2) and (3) cannot all be satisfied if X is a configuration of densely packed hard-sphere particles. Hence the idea is to construct a transformation $\mathfrak{T}_n$ with some of these

properties, namely (2),(3) and (4) and then to show that $\mathfrak{T}_n$ also has the other properties for all X from a set of good configurations G_n of probability close to 1. The construction of $\mathfrak{T}_n$ can be given in a natural way by a recursive modification of the independent transformation mentioned above, where the hard core condition is implemented by local distortions around particles already considered. The set G_n can be described in terms of geometric properties of the configurations. For example, condition (1) can be seen to be equivalent with the statement that a certain percolation cluster starting from a neighbourhood of the origin is bounded, which can be shown to have probability close to 1 if n is chosen big enough. Similar arguments can be applied to other properties required of good configurations.

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The Allen-Cahn Action functional in higher dimensions

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(joint work with Luca Mugnai)

The (renormalized) *Allen–Cahn action functional* is given by

$$\mathcal{S}_\varepsilon(u) := \int_0^T \int_\Omega \Big(\sqrt{\varepsilon}\partial_t u + \frac{1}{\sqrt{\varepsilon}}\big(-\varepsilon\Delta u + \frac{1}{\varepsilon}W'(u)\big)\Big)^2 \, dx\, dt.$$

This functional arises in the analysis of the stochastically perturbed Allen–Cahn equation and is, by large deviation theory, related to the probability of rare events. Kohn, Reznikoff, and Tonegawa [3] and Kohn, Otto, Reznikoff, and Vanden–Eijnden [2] suggested a *reduced action functional* in the sharp interface limit $\varepsilon \to 0$. For phase indicator functions $u : (0,T) \times \Omega \to \{-1,1\}$ such that $\partial\{u = 1\} \cap \Omega$ is apart from a countable set of singular times given as smooth evolution of smooth hypersurfaces $\Sigma := \cup_{t\in(0,T)}\{t\} \times \Sigma_t$ the reduced action is defined by

$$\mathcal{S}_0(u) := c_0 \int_0^T \int_{\Sigma_t} \big|v(t,\cdot) - H(t,\cdot)\big|^2 \, d\mathcal{H}^{n-1}dt \; + 8c_0 \sum_i \mathcal{H}^{n-1}(\Sigma_i).$$

Here Σ_i denotes the i^{th} component of Σ at the time of creation, v denotes the normal velocity of the evolution $(\Sigma_t)_{t\in(0,T)}$, $H(t,\cdot)$ denotes the mean curvature

vector of Σ_t, and $c_0 := \int_{-1}^{1} \sqrt{2W}$. In [2] lower and upper bounds that match in terms of scaling were constructed and the lower estimate was shown for sequences $(u_\varepsilon)_{\varepsilon>0}$ such that the associated 'energy-measures' have *equipartitioned energy* and *single multiplicity* as $\varepsilon \to 0$.

Our goal is a compactness result for sequences with uniformly bounded action and a sharp lower-bound of the functional $\mathcal{S}_\varepsilon$ in space dimensions $n = 2, 3$ without any additional restrictions on the approximate sequences. To circumvent problems with cancellations of interfaces we analyze the limit of the diffuse energy measures and generalize the reduced action functional $\mathcal{S}_0$ to a suitable class of *evolving measures*. In particular we introduce a generalized formulation of velocity.

Definition 1. *Let Ω be an open bounded subset of $\mathbb{R}^n$, $T > 0$ and $\Omega_T := (0,T)\times\Omega$. Choose W to be the quartic double-well potential $W(r) = \frac{1}{4}(1-r^2)^2$. We define for $\varepsilon > 0$, $t \in (0,T)$, the* energy measures

$$\mu_\varepsilon^t := \Big(\frac{\varepsilon}{2}|\nabla u_\varepsilon|^2(t,\cdot) + \frac{1}{\varepsilon}W(u_\varepsilon(t,\cdot))\Big)\mathcal{L}^n.$$

Assumption 1. *Let $n = 2, 3$ and let a sequence $(u_\varepsilon)_{\varepsilon>0}$ of smooth functions be given that satisfies for all $\varepsilon > 0$*

$$\mathcal{S}_\varepsilon(u_\varepsilon) \le \Lambda, \tag{1}$$

$$u_\varepsilon(0,\cdot) = -1, \qquad u_\varepsilon(T,\cdot) = 1, \tag{2}$$

$$\nabla u_\varepsilon \cdot \nu_\Omega = 0 \quad \text{on } [0,T]\times\partial\Omega. \tag{3}$$

The restriction to the 'switching scenario' (2) is for simplicity and not essential for our analysis. The uniform bound on the action and (2), (3) imply that

$$\int_{\Omega_T} \Big(\varepsilon(\partial_t u_\varepsilon)^2 + \frac{1}{\varepsilon}\big(-\varepsilon\Delta u_\varepsilon + \frac{1}{\varepsilon}W'(u_\varepsilon)\big)^2\Big)\,d\mathcal{L}^{n+1} + 2\max_{0\le t\le T}\mu_\varepsilon^t(\Omega) \le \Lambda.$$

The first Proposition is an application of [4].

Proposition 8. *There exists $u \in BV(\Omega_T,\{-1,1\}) \cap L^\infty(0,T;BV(\Omega))$ such that for a subsequence $\varepsilon \to 0$*

$$u_\varepsilon \to u \qquad \text{in } L^1(\Omega_T),$$
$$u_\varepsilon(t,\cdot) \to u(t,\cdot) \qquad \text{in } L^1(\Omega) \text{ for almost all } t \in (0,T).$$

Next we basically repeat [3, Theorem 1.1].

Proposition 9. *There exists a countable set $S \subset (0,T)$, a subsequence $\varepsilon \to 0$, and Radon measures $\mu^t, t \in [0,T]\setminus S$, such that for all $t \in [0,T]\setminus S$*

$$\mu_\varepsilon^t \to \mu^t \text{ as Radon measures on } \overline{\Omega},$$

such that $\mu_\varepsilon^t\,dt \to \mu^t\,dt$, and such that for all $\psi \in C^1(\overline{\Omega})$ the map $t \mapsto \mu^t(\psi)$ is of bounded variation in $(0,T)$ and has no jumps in $(0,T)\setminus S$.

We use the lower bound [5] to prove that the measures μ^t are up to a constant integer-rectifiable with a weak mean curvature satisfying an appropriate lower estimate.

Theorem 10. *For almost all $t \in (0,T)$ we obtain that $c_0^{-1}\mu^t$ is an integral $(n-1)$-varifold, that μ^t has weak mean curvature $H(t,\cdot) \in L^2(\mu^t)$, and that*

$$\int_0^T \int_\Omega |H(t,\cdot)|^2 \, d\mu^t \, dt \;\le\; \liminf_{\varepsilon\to 0} \int_{\Omega_T} \frac{1}{\varepsilon}\Big(-\varepsilon\Delta u_\varepsilon + \frac{1}{\varepsilon} W'(u_\varepsilon)\Big)^2 \, d\mathcal{L}^{n+1}.$$

We next obtain the existence of a generalized velocity of $(\mu^t)_{t\in(0,T)}$.

Theorem 11. *Let $(\mu^t)_{t\in(0,T)}$ be the limit measures obtained in Proposition 9. Then there exists a vector field $v \in L^2(\mu, \mathbb{R}^n)$ that satisfies*

$$\sup_\eta \Big\{ \Big| \int_0^T \int_\Omega \big(\partial_t \eta + \nabla\eta^\perp \cdot v\big)\, d\mu^t dt \Big| \;:\; \eta \in C_c^1((0,T)\times\overline{\Omega}), |\eta| \le 1 \Big\} \;<\; \infty. \tag{4}$$

Moreover we have the lower bound

$$\int_{\Omega_T} |v|^2 \, d\mu \;\le\; \liminf_{\varepsilon\to 0} \int_{\Omega_T} \varepsilon(\partial_t u_\varepsilon)^2 \, d\mathcal{L}^{n+1}.$$

We also prove that (4) determines uniquely the normal component of v in almost all points where μ is rectifiable and that v gives the distributional derivative of the phases in the sense that for all $\eta \in C_c^1(\Omega_T)$

$$\int_0^T \int_\Omega v(t,x) \cdot \frac{\nabla u}{|\nabla u|}(t,x)\eta(t,x)\, d|\nabla u(t,\cdot)|(x) dt \;=\; -\int_{\Omega_T} u\partial_t\eta \, d\mathcal{L}^{n+1}.$$

As our main result we obtain the lower estimate for $\mathcal{S}_\varepsilon$.

Theorem 12. *Let Assumption 1 hold, and let $(\mu^t)_{t\in[0,T]}$ and S be as in Proposition 9. Define the* nucleation cost $\mathcal{S}_{nuc}(\mu)$ *by*

$$\mathcal{S}_{nuc}(\mu) \;:=\; \sum_{t_0\in S} \sup_\psi \Big(\lim_{t\downarrow t_0} \mu^t(\psi) - \lim_{t\uparrow t_0} \mu^t(\psi)\Big) + \sup_\psi \lim_{t\downarrow 0} \mu^t(\psi),$$

where the sup *is taken over all $\psi \in C^1(\overline{\Omega})$ with $0 \le \psi \le 1$. Then*

$$\liminf_{\varepsilon\to 0} \mathcal{S}_\varepsilon(u_\varepsilon) \;\ge\; \int_{\Omega_T} |v - H|^2 \, d\mu + 4\mathcal{S}_{nuc}(\mu).$$

For the proof of our results we use tools from Geometric Measure Theory, in particular varifold theory, arguments from [5], and the measure–function pair convergence introduced by Hutchinson [1]. As in [5] the *equipartitioning of energy* in the limit $\varepsilon \to 0$ is one important property that has to be proved. We consider the diffuse velocity vectors v_ε and diffuse mean curvatures H_ε defined by

$$v_\varepsilon \;:=\; -\frac{\partial_t u_\varepsilon}{|\nabla u_\varepsilon|}\frac{\nabla u_\varepsilon}{|\nabla u_\varepsilon|}, \qquad H_\varepsilon \;:=\; \frac{1}{\varepsilon} w_\varepsilon \frac{\nabla u_\varepsilon}{|\nabla u_\varepsilon|^2}.$$

We then show that

$$\begin{aligned} (\varepsilon|\nabla u_\varepsilon|^2 d\mathcal{L}^{n+1}, H_\varepsilon) \;&\to\; (\mu^t dt, H),\\ (\varepsilon|\nabla u_\varepsilon|^2 d\mathcal{L}^{n+1}, v_\varepsilon) \;&\to\; (\mu^t dt, v) \end{aligned}$$

in the sense of measure-function-pair convergence. From this result we deduce the lower estimates of the mean curvature and generalized velocity, and derive

the equation (4) that identifies v as a velocity in a generalized sense. Our results allow us to conclude the Gamma convergence of $\mathcal{S}_\varepsilon$ to a relaxed version of $\mathcal{S}_0$ in a restricted class of 'nice' indicator functions. To achieve a full Gamma-convergence result one has in particular to analyze the class of function for which the *limsup*-estimate can be derived. For a precise statement of our results and details of the proofs we refer to [6].

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Elastic-ideally plastic beams and 1D Prandtl–Ishlinskii hysteresis operators

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(joint work with Pavel Krejčí)

This note is concerned with modeling small strain transversal oscillations of lower-dimensional mechanical structures. Here, we confine ourselves to one-dimensional beams that have been studied in [6], [7]; corresponding results for elastoplastic Kirchhoff plates have recently been established in [3]. The aim of this study is to demonstrate that there are close connections between two seemingly quite different models for elastoplasticity: the *von Mises plasticity criterion*, which is frequently used by engineers, and the hysteresis model that was introduced in [8], [4], and is known as the *Prandtl–Ishlinskii hysteresis operator*.

The surprising result of the analysis is that, using the classical scaling hypotheses that can be found in [2], the three-dimensional single-yield von Mises approach leads after the dimensional reduction to a one-dimensional multi-yield Prandtl–Ishlinskii hysteresis operator. This can be explained by the fact that in the 1D model only deformations of longitudinal fibers parametrized by the transversal coordinate are taken into account, and the individual fibers do not switch from the elastic to the plastic regime simultaneously; more precisely, the eccentric fibers look alike as if they had a higher modulus of elasticity and lower yield points than the central ones. Another surprise is that the weight function of the Prandtl–Ishlinskii operator can be *explicitly determined*; this fact is particularly relevant

from the viewpoint of applications, since previously the practical use of Prandtl–Ishlinskii operators in elastoplasticity was hampered by the fact that their weight functions had to be identified from measurements.

More specifically, it turns out from the analysis that the small strain transversal oscillations of a one-dimensional beam of length $L > 0$ can be described as a partial differential equation of the form

$$\rho\, w_{tt} - \frac{\rho\, h^2}{3}\, w_{xxtt} + \mathcal{P}[w_{xx}]_{xx} = g \quad \text{in } (0,L)\times(0,T)\,. \tag{1}$$

Here, $\rho > 0$ is the mass density, $2h > 0$ the thickness of the beam, g the distributed load, and $\mathcal{P}$ a Prandtl–Ishlinskii operator of the form

$$\mathcal{P}[v](t) = \int_{\frac{R^3}{E^2\, h}}^{\infty} q^{-4}\, \mathcal{S}_q[v](t)\, dq\,. \tag{2}$$

In this formula, $R > 0$ stands for the yield limit of the von Mises plasticity criterion, E is Young's modulus, and $\mathcal{S}_q$ is the *stop operator with thresholds* $\pm q$, which is defined as follows: it is well known (see [5]) that for every input function $v \in W^{1,1}(0,T)$ and every initial value $\chi_0 \in [-q,+q]$ there is a unique solution $\chi \in W^{1,1}(0,T)$ to the variational inequality

$$\begin{aligned} &\chi(t) \in [-q,+q] \quad \forall\, t \in [0,T]\,, \quad \chi(0) = \chi_0\,, \\ &(\dot\chi(t) - \dot v(t), \chi(t) - w) \le 0 \quad \text{a.e. in } (0,T)\,, \quad \forall\, w \in [-q,+q]\,. \end{aligned} \tag{3}$$

The solution operator

$$\mathcal{S}_q : [-q,+q]\times W^{1,1}(0,T) \to W^{1,1}(0,T);\ \ (\chi_0, v) \mapsto \chi\,,$$

is just the stop operator with thresholds $\pm q$. In the terminology of elastoplasticity, it is also called *Prandtl's elastic-ideally plastic element*. It is well known (see [1], [5]) that $\mathcal{S}_q$ can be extended by a density argument for fixed initial datum $\chi_0 \in [-q,+q]$ to a globally Lipschitz continuous mapping from $C[0,T]$ into itself. Moreover, the operator $\mathcal{S}_q$ enjoys the *dissipation property* (see [1], [5]):

$$\frac{1}{2}\frac{d}{dt}\big(\mathcal{S}_q[v](t)\big)^2 \le \mathcal{S}_q[v](t)\,\dot v(t) \quad \text{a.e. in } (0,T)\,, \quad \forall\, v \in W^{1,1}(0,T)\,. \tag{4}$$

In addition to that, it holds the *second-order energy estimate* (which follows from the fact that the hysteresis loops generated by the stop operator are convex), cf. [1], [5]):

$$\frac{d}{dt}\mathcal{S}_q[v](t)\,\ddot v(t) \le \frac{d}{dt}\left(\frac{1}{2}\frac{d}{dt}\mathcal{S}_q[v](t)\,\dot v(t)\right) \ \text{ a.e. in } (0,T)\,,\ \forall\, v \in W^{2,1}(0,T)\,, \tag{5}$$

in the sense of distributions. The above inequalities are of fundamental importance to show that certain initial-boundary value problems associated with the above partial differential equation admit a unique solution. For a detailed statement and proof of these results, we refer to the papers [6], [7], [3]. In these papers, also a complete account of the corresponding modeling issues is given.

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Elastic biomembranes with lateral phase separation

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(joint work with Charles M. Elliott)

Subject of our research are bi-layer lipid membranes with coexisting intermembrane domains. The energy of such membranes involves an elastic bending part and a line part arising from the boundaries of the different fluid domains. Current approaches go back to works of Canham, Evans, and Helfrich (see for example [2]) and model the membrane as a smooth hypersurface $\Gamma \subset \mathbb{R}^3$. To leading order an elastic energy is of the form

$$F_{\text{bending}} = \int_\Gamma \frac{k}{2}(\kappa - \bar{\kappa})^2.$$

Here, k is the bending rigidity, κ the curvature, and $\bar{\kappa}$ a given spontaneous curvature. Intermembrane domains separating two phases with different lipid composition have been considered by Jülicher and Lipowsky [4]. In their model the domains are separated by smooth curves γ on the membrane, and the line energy is given by $F_{\text{line}} = \int_\gamma \sigma$ with a line energy density coefficient σ.

In biophysics, equilibrium shapes of membranes with sphere-like topology are of interest in dependence of the total membrane area $|\Gamma|$, the volume of the enclosed domain, the surface area ratio of the two phases, and the coefficients k, $\bar{\kappa}$, and σ. So far existing analytical studies [4, 3] are restricted to (more or less) symmetric cases. Numerical studies are restricted to membranes close to a sphere [5] or are based on diffuse interface models for the membrane [1]. Our goal has therefore been to provide a numerical tool based on a finite element discretization of the membrane in order to study (local) minima or, respectively, the gradient flow dynamics of the membrane energy.

For the phase separation a diffuse interface approach has been applied. An order parameter $c : \Gamma \to [0,1] \subset \mathbb{R}$ represents one of the phases. The line energy is replaced by a Ginzburg- Landau functional

$$F_{\mathrm{GL}} = \int_\Gamma f, \quad f = \frac{\sigma\varepsilon}{2}|\nabla_\Gamma c|^2 + \frac{\sigma}{\varepsilon}\psi(c)$$

where ∇_Γ stands for the surface gradient and $\psi(c)$ is a double-well potential with minima in 0 and 1 corresponding to the two phases. The constraint on the surface area ratio of the two phases becomes a constraint of the form $\int_\Gamma h(c)$ with a monotone function h satisfying $h(0) = 0$, $h(1) = 1$, and $h'(0) = h'(1) = 0$.

In order to set up the gradient flow dynamics we need a variation of the energy with respect to Γ which is based on a deformation of the domain with a vector field $\boldsymbol{w}$. Setting $\boldsymbol{y} = (\kappa - \bar\kappa)\boldsymbol{\nu}$ with the unit normal $\boldsymbol{\nu}$ on Γ the variation of the bending part of the energy is $\langle \delta_\Gamma F_{\mathrm{bending}}, \boldsymbol{w}\rangle = \int_\Gamma (\frac{k}{2}|\boldsymbol{y}|^2 \nabla_\Gamma \cdot \boldsymbol{w} + \partial_\tau^\bullet \boldsymbol{y} \cdot \boldsymbol{y})$ where $\partial_\tau^\bullet$ can be seen as material derivative when interpreting $\boldsymbol{w}$ as velocity field and the deformation parameter τ as time. To compute the last term an idea of Dziuk has been used. Denoting by $\boldsymbol{x} : \Gamma \to \Gamma$ the identity and by Δ_Γ the surface Laplacian the curvature vector fulfills the identity $\kappa\boldsymbol{\nu} = \Delta_\Gamma \boldsymbol{x}$. Hence for test functions $\boldsymbol{b}$

$$0 = \int_\Gamma \boldsymbol{y} \cdot \boldsymbol{b} + \nabla_\Gamma \boldsymbol{x} : \nabla_\Gamma \boldsymbol{b} + \bar\kappa \boldsymbol{\nu} \cdot \boldsymbol{b},$$

which also holds on the deformed membranes. Differentiating this identity with respect to the deformation parameter τ and, after, replacing $\boldsymbol{b}$ by $\boldsymbol{y}$ yields an identity for the term $\int_\Gamma \partial_\tau^\bullet \boldsymbol{y} \cdot \boldsymbol{y}$.

To compute the variation of the Ginzburg-Landau energy with respect to Γ it turns out to be necessary to state a law for $\partial_\tau^\bullet c$. The simplest case would be to demand no changes to c when deforming Γ, but the value $\int_\Gamma h(c)$ needs to be kept constant. This is taken into account with a Lagrange multiplier, hence $\partial_\tau^\bullet c := -\lambda_c h'(c)$ with $\lambda_c = \int_\Gamma h(c)\nabla_\Gamma \cdot \boldsymbol{w} / \int_\Gamma (h'(c))^2$.

The evolution of the surface is defined by the L^2 gradient flow, taking the constraints C_A on surface area and C_V on enclosed volume with Lagrange multipliers into account. This results in

$$\begin{aligned}
\int_\Gamma \partial_t \boldsymbol{x} \cdot \boldsymbol{w} = &- k \int_\Gamma -\frac{1}{2}|\boldsymbol{y}|^2 \nabla_\Gamma \cdot \boldsymbol{w} - \nabla_\Gamma \cdot \boldsymbol{y}\, \nabla_\Gamma \cdot \boldsymbol{w} - \nabla_\Gamma \boldsymbol{y} : \nabla_\Gamma \boldsymbol{w} \\
&- k \int_\Gamma (\nabla_\Gamma \boldsymbol{y})^\perp : \nabla_\Gamma \boldsymbol{w} + \boldsymbol{P}\nabla_\Gamma \boldsymbol{y} : \nabla_\Gamma \boldsymbol{w} \\
&- k \int_\Gamma -\bar\kappa\big(\nabla_\Gamma \cdot \boldsymbol{y}\, \boldsymbol{n} \cdot \boldsymbol{w} - \nabla_\Gamma \boldsymbol{y} : \boldsymbol{n} \otimes \boldsymbol{w}\big) \\
&- \int_\Gamma \Big(\frac{-\int \mu h'(c)}{\int (h'(c))^2} h(c) + f\Big)\nabla_\Gamma \cdot \boldsymbol{w} - \sigma\varepsilon \nabla_\Gamma c \otimes \nabla_\Gamma c : \nabla_\Gamma \boldsymbol{w} \\
&- \lambda_V \int_\Gamma \boldsymbol{n} \cdot \boldsymbol{w} - \lambda_A \int_\Gamma \boldsymbol{\kappa} \cdot \boldsymbol{w}.
\end{aligned}$$

Here, the potential

$$\mu = \delta_c F_{\mathrm{GL}} = -\sigma\varepsilon\Delta_\Gamma c + \frac{\sigma}{\varepsilon}\psi'(c)$$

appears. It is also used to define the evolution of the order parameter c:

$$\partial_t^\bullet c := -K\mu - \lambda_c h'(c)$$

where again a Lagrange multiplier appears subject to keeping $\int_\Gamma h(c)$ constant. The above equations is of Allen-Cahn type with an additional forcing term due to the constraint.

It can be shown that the membrane energy indeed decreases. It holds that

$$0 = \int_\Gamma |\partial_t \boldsymbol{x}|^2 + \frac{d}{dt}\big(F_{\mathrm{bending}} + F_{\mathrm{GL}}\big) + \int_\Gamma \frac{K}{2}\big(\mu - \lambda_\mu h'(c)\big)^2 + \frac{\sigma}{2K}\big(\partial_t^\bullet c - \lambda_{\boldsymbol{v}} h'(c)\big)^2$$

where $\lambda_\mu = \int(\mu h'(c))/\int(h'(c))^2$ and $\lambda_{\boldsymbol{v}} = \int(\partial_t^\bullet c\, h'(c))/\int(h'(c))^2$.

There are certainly other possibilities to define the evolution of the order parameter such that the energy decreases and the ratio of the phase areas is maintained, e.g., an evolution according to a Cahn-Hilliard type equation, c being a conserved quantity. Since we only have a restriction to the total surface area of the membrane the surface can locally stretch or compress. In a pure phase, i.e., c constant close to 0 or 1, a conserved order parameter would develop gradients, whence also line energy contributions appear in the pure phases. This has a re-impact on the evolution of the surface, and in numerical simulation we observed that the mesh properties became very worse necessitating a rearrangement of the grid points. Such effects can be avoided by trying to maintain the value of c in the pure phases which motivates the above setup. In particular, the choice of h with the properties $h'(0) = h'(1) = 0$ ensures that an adaption of c to keep $\int_\Gamma h(c)$ constant only takes place in the interfacial regions.

The presented approach is easily accessible to a discretization with linear finite elements since only first order derivatives appear in the governing equations. The new approach for the bending energy based on Dziuk's idea leads to an astonishing good mesh behavior. In the example in Fig. 1 the membrane suffers a drastic deformation without requiring any re-meshing.

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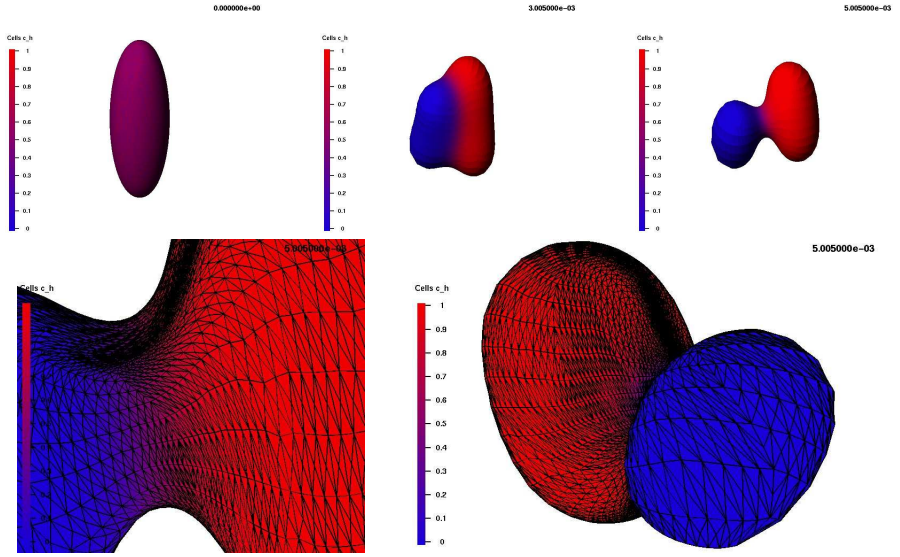

FIGURE 1. Evolution of a prolate membrane with random initial field c. The deformation is drastic but a rearrangement of the vertexes was not necessary. The lower figures show the mesh at the final time revealing some very elongated triangles in the neck region. In the pure phase the triangles should be refined.

Long-time validity of the gainless homogeneous Boltzmann equation

FLORIAN THEIL
(joint work with Karsten Matthies)

This paper introduces new results which establish the validity of a continuum description for the deterministic dynamics of many interacting particles. Here the many particle evolution is analyzed for a hard sphere flow with the addition that after a collision the collided particles are removed from the system (ballistic annihilation). The initial conditions are assumed to be iid random variables whose law is a spatially homogeneous velocity density $f_0(v)$ that has finite mass and variance (kinetic energy) and does not concentrate mass on lines. Under these assumptions it is proven rigorously in that in the Boltzmann-Grad limit the evolution of the particle density is described by the homogenous Boltzmann equation without gain term for arbitrary long times.

We consider a simplified version of hard-ball dynamics where n balls with diameter $a > 0$ move along straight lines until they collide and are removed after the collision. This case is usually referred to as *ballistic annihilation*. The initial positions of the centers of the balls $(u_0(i), v_0(i)) \in \mathbb{T}^d \times \mathbb{R}^d$, $i = 1 \dots n$ are iid random variables with law $1_{\mathbb{T}^d} \otimes f_0 \in PM(\mathbb{T}^d \times \mathbb{R}^d)$. We send n to infinity and prove rigorously that the weak-* limit of the empirical densities satisfies a simple

mean-field theory, *provided* that $f_0 \in M_+(\mathbb{R}^d)$ has finite total mass and kinetic energy

$$\int_{\mathbb{R}^d} (1+|v|)^2 \,\mathrm{d}f_0(v) = K < \infty \tag{1}$$

and does not concentrate mass on single velocity directions, i.e.

$$\int_{\rho(v,\nu)} \mathrm{d}f_0(v') = 0 \text{ for all } v \in \mathbb{R}^d, \nu \in S^{d-1}, \tag{2}$$

where $\rho(v,\nu) = v + \mathbb{R}\,\nu$. Assumption (2) seems to be new. If the initial distribution f_0 satisfies assumptions (1) and (2), then as the particle number n tends to infinity, the particle density converges to a solution of the Boltzmann equation (Theorem 13). On the other hand, if assumption (2) is not satisfied, then it cannot be expected that the particle density converges to a solution of the Boltzmann equation, cf Theorem 14.

The kinetic annihilation dynamics has attracted considerable attention for two reasons. It models some growth and coarsening processes [KS88] and in some cases can be can be solved exactly. The questions we are asking have been addressed before, mainly in the physics-literature. It is well-known that if $d = 1$ the kinetic annihilation dynamics cannot be described by a simple Boltzmann-type mean-field theory, cf [EF85]. A derivation (based on the BBGKY-hierarchy) of the gainless Boltzmann equation as a scaling limit of the annihilation dynamics can be found in [PTD02], however no explicit assumption concerning the regularity of the initial distribution f_0 is made. Hence, our Theorem 14 would constitute a counterexample.

Theorem 13. *(Justification of the gainless Boltzmann equation)*
Let $f_0 \in PM_+(\mathbb{R}^d)$, $d \geq 2$ be a momentum density that satisfies (1, 2) and let for each $N \in \mathbb{N}$ the initial values $(u_0(i), v_0(i))$, $i = 1 \ldots n$ be such that $\omega = \{(u_0(i), v_0(i)) \,|\, i = 1 \ldots n\} \subset \mathbb{T}^d \times \mathbb{R}^d$ is a Poisson point process with intensity $N(\mathbf{1}_{\mathbb{T}^d} \otimes f_0)$. Let $u_t(i) = u_0(i) + tv_0(i)$, $v_t(i) = v_0(i)$ and $\beta_t(i) \in \{0,1\}$ be the indicator function of particles that haven't collided yet. If the diameter of the particles a depends on N such that

$$Na^{d-1} = 1,$$

then for each $t \in [0,\infty)$, $\varepsilon > 0$, measurable $\Omega \subset \mathbb{T}^d \times \mathbb{R}^d$

$$\lim_{N\to\infty} \mathrm{Prob}\Bigg(\bigg| \frac{1}{N} \# \Big\{ i \in \{1 \ldots n\} \mid (u_t^{(N)}(i), v_t^{(N)}(i)) \in \Omega \text{ and } \beta_t^{(N)}(i) = 1 \Big\} - \int_\Omega \mathrm{d}u \,\mathrm{d}f_t(v) \bigg| > \varepsilon \Bigg) = 0,$$

where $f : [0,\infty) \to M_+(\mathbb{R}^d)$ is the unique solution of the gainless, homogeneous Boltzmann equation

$$\dot{f} = Q_-[f,f], \quad f_{t=0} = f_0, \tag{3}$$

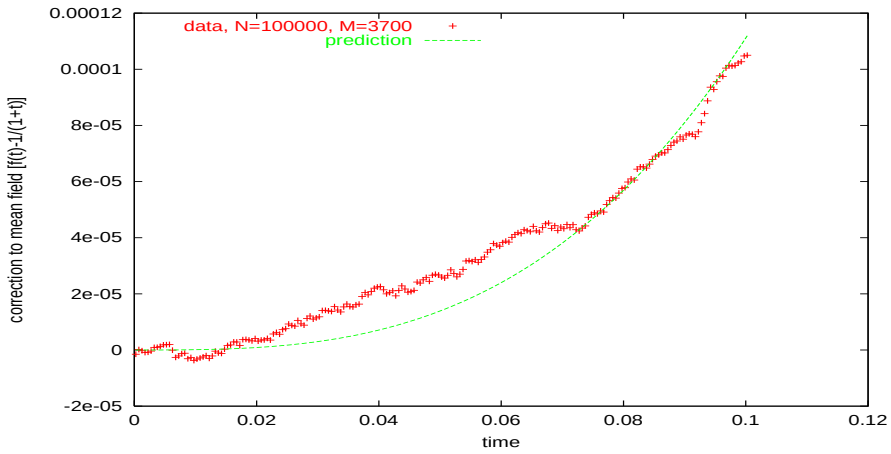

FIGURE 1. Comparison between the empirical probability of colliding and the mean-field prediction. The dashed line is the cubic parabola $t \mapsto \frac{1}{9}t^3$, the signs '+' mark the difference between the number of non-collided particles at time t divided by N and the mean-field prediction $\frac{1}{1+t}$.

and $Q_-[f,f](v) = -\int_{\mathbb{R}^d} \mathrm{d}f(v')\,\kappa_d|v-v'|\,f(v)$ *is the loss term. The number* κ_d *is the volume of* $d-1$ *dimensional unit-ball, in particular* $\kappa_2 = 2, \kappa_3 = \pi$.

We illustrate that the mean field theory does not capture the many-particle dynamics if the initial distribution f_0 exhibits strong concentrations and violates (2). Explicit results can be obtained for $d = 2$, but a similar phenomena are expected to hold in the case $d = 3$.

Theorem 14. *Let* $v \in \mathbb{R}^2$ *be nonresonant* ($\alpha \cdot v \notin \mathbb{Z}$ *for all* $\alpha \in \mathbb{Z}^d$) *such that* $|v| = \frac{1}{4}$ *and set* $f_0 = \frac{1}{2}(\delta(\cdot - v) + \delta(\cdot + v))$. *If* $\hat{Q}(t) = \lim_{k,N\to\infty} \mathrm{Prob}(\beta_t(1) = 1)$ *denotes the empirical probability that a tagged particle does not collide, then*

$$\lim_{t\to 0} \frac{1}{t^3} \left| \int_{\mathbb{R}^2} \mathrm{d}f_t(v) - \hat{Q}(t) \right| = \frac{1}{9}, \tag{4}$$

where $f_t = \frac{1}{1+t} f_0$ *is the unique solution of the Boltzmann equation (3) which satisfies the initial condition* $f_{t=0} = f_0$.

A numerical simulation (fig. 1) confirms the prediction (4).

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Rate independent plasticity and criticality

Lev Truskinovsky

Singular dissipative potential of the phenomenological rate independent plasticity is obtained by homogenization of a micro-model with quadratic dissipation. The essential ingredient making this reduction possible is a rugged energy landscape at the micro-scale, generating under external loading a regular cascade of subcritical bifurcations. Such landscape appear as a result of a sufficiently strong pinning or jamming of defects. The criticality of the resulting process is revealed by the power law acoustic emission.

The main objective of this resume, summarizing some recent results obtained in collaboration with A. Vainchtein, G. Puglisi, F. J, Pérez-Reche and. G. Zanzotto, is to demonstrate that classical plasticity can be derived from a model with viscous dissipation as a result of a judicial elimination of small spatial scales and fast times. The singular dissipative structure emerges in this approach as a consequence of time averaging and spatial homogenization in a system with regular dissipative behavior. The main idea, which dates back to L. Prandtl, is to consider rate independence as a limit of rate dependence with zero and unbounded strain rates finely mixed.

Experimentalists know that during quasi-static plastic deformation of metals the dislocation dynamics is not continuous but intermittent in space and time with rest periods interrupted by brief moments of energetic activity. During these isolated bursts, associated with depinning or nucleation of defect micro-structures, the instantaneous strain rate may exceed the imposed strain rate by several orders of magnitude. Since practically all conversion of mechanical energy into heat takes place during these fast events, the overall dissipation depends only on the number of unstable episodes which is invariant under time re- parametrization. The physical picture behind the quasi-static behavior of shape memory alloys is similar with a replacement of a dislocation by a phase or domain boundary as a carrier of an inelastic deformation.

To illustrate the general idea we analyze in some detail a simple mechanical system whose microscopic dynamics is of a gradient flow type and whose homogenized macroscopic behavior is rate independent plastic. The basis of the model is a one dimensional lattice of interacting elastic elements with non-convex energies; the analytic transparency is due to the (mean field type) assumption that the elements interact exclusively through the average strain. The elemental bi-stability reflects the presence of two states – jammed and released; an additional assumption of piece-wise linearity allows for an explicit separation of the motion into adiabatic and jump parts. The main conceptual limitation of this preliminary model is its low-dimensionality and the neglect of disorder.

We then show that the uneven distribution of the elemental metastability thresholds produces hardening and replaces already in 2D a regular stick slip motion with a random distribution of avalanches revealed by power-law- distributed acoustic signals. We illustrate those effect with an example of a rate independent hysteresis associated with transformational plasticity in martensites. During

martensitic phase transformations the macroscopic discontinuity of the order parameter typically splits into a set of bursts indicating transitions between neighboring metastable states. The individual avalanches can be detected through the measurement of the intermittent acoustic and calorimetric signals. For instance, experiments in Cu-based memory alloys (CuAlNi, CuZnAl, CuAlMn) show that the amplitudes of these avalanches exhibit a power-law distribution. The steady state hysteresis profile with critical properties emerges in these systems only after multiple thermal cycling through the transition.

In spite of the substantial theoretical effort, the process of self- organization towards a scale-free behavior in martensites, emphasized by the necessity of 'training' for these materials, has never been fully understood. By applying our model we were able to show that the dislocation activity is a crucial factor of this self organization. We developed a 2D extension of the model which incorporates the intrinsic periodicity of the energy landscape and allows one to deal simultaneously with phase boundaries and dislocations. From this basis we derived a self-organizing discrete model with threshold dynamics, equivalent to a sandpile automaton. Despite its ultimate simplicity, the model reproduces all principal observations in thermally and mechanically cycled martensites including training induced power-law behavior, plastic shakedown, characteristic asymmetry of the acoustic signals and the absence of the scaling collapse. The model predicts self organized development of the highly correlated disorder which the system retains after full unloading.

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Rigid interfaces via Reflection Positivity

Yvon Vignaud

(joint work with Senya Shlosman)

Since the seminal work of Dobrushin [2] on the interface of 3D Ising model at low temperature in 1972, several results on rigid interfaces have been rigorously obtained for various models. In a joint work with Senya Shlosman we used the method of Reflection Positivity to derive such results for a model with infinitely many ground states.

I will start by giving the motivations which led us to study such a model and briefly recall the state of the art as regards rigid interfaces and Dobrushin states. Then I will state our result and explain the main line of the proof. It is remarkable that our method actually applies to Ising and Potts models, leading to drastic

simplifications in the proofs which used cluster expansions techniques. All models below are considered on the lattice $\mathbb{Z}^d$ whose edges are denoted $\langle i, j\rangle$.

1. Motivations and known results

The main result of Dobrushin's paper [2] is the construction of a Gibbs state which describes the coexistence of phases in 3D Ising model at low temperatures. In such a state, the configurations exhibit a rigid interface separating the plus phase from the minus phase; this interface is a deterministic horizontal plane with small random perturbations.

Such states have been constructed for other models. Namely,

- critical Potts model for high q (Messager *et al.*, 1991) [6]
- supercritical bond percolation (Gielis–Grimmett, 2002) [5]
- critical random-cluster model (Černý–Kotecký, 2003) [1]

These models have in common that their symmetry group is discrete. Since some models with continuous symmetry exhibit phase transition as well [4], it is relevant to ask the following question: is it possible to construct Dobrushin states for a 3D model with continuous symmetry? We conjecture that it is indeed possible, and suggest the following Hamiltonian as a plausible candidate:

$$H(\sigma) = \sum_{\langle i,j\rangle} U(|\sigma_i - \sigma_j|), \tag{1}$$

where spins σ_i take values in the circle $\mathbb{S}^1 = \mathbb{R}_{/\mathbb{Z}}$ and $U(r) = -\left(\frac{1+\cos r}{2}\right)^p$, p being a large integer. In [7, 8], the auhors proved that this model undergoes a phase transition from order to disorder provided that the dimension of the lattice is at least two. We conjecture that the interface between the ordered phase and the disordered phase of the model (1) is rigid when $d \geq 3$.

2. New results

In this section we present our results, which support the conjecture above. The first result derives the rigidity property of an order/disorder interface for a toy model of the model (1), in a partial thermodynamic limit. The second result derives the rigidity property for a clock version of the toy model, in the full thermodynamic limit.

We fix a (small) parameter $\varepsilon > 0$ and consider the toy model given by the following Hamiltonian

$$H(\sigma) = \sum_{\langle i,j\rangle} U(|\sigma_i - \sigma_j|), \tag{2}$$

where spins σ_i take values in $\mathbb{S}^1$ and $U(r) = -\mathbb{1}_{\{r\leq\varepsilon\}}$.

The clock version of this toy model is given by the following Hamiltonian

$$H(\sigma) = \sum_{\langle i,j\rangle} U(|\sigma_i - \sigma_j|), \tag{3}$$

where spins σ_i take values in $\mathbb{Z}_{/q\mathbb{Z}}$ and $U(r) = -\mathbb{1}_{\{r\leq 1\}}$, q being a (large) positive integer.

A straightforward adaption of the techniques developed in [7, 8] shows that when $d \geq 2$, both models undergo a first-order phase transition between order and disorder, provided that $\varepsilon < \varepsilon_0(d)$ and $q > q_0(d)$ respectively.

Considering any configuration σ with ordered b.c. on the top of our box, disordered b.c. on the bottom and periodic b.c. on vertical boundaries, it is possible to define the order–disorder interface $I(\sigma)$, which is a (random) object separating a disordered phase (below) from and ordered phase (above). In a standard way, one can define *ceilings* of I as the "flat pieces" of I. The *rigidity set* of I is the ceiling of I with largest area; we denote it by $R = R(I(\sigma))$.

Denoting by $\mu_{N,L}$ the Gibbs measure in the box $\Lambda_{N,L}$ with the b.c. described above and at coexistence temperature $T = T_c$, our main result is the following:

Theorem 15 ($d = 3$)**.**

- *If $\varepsilon < \varepsilon_1$ then there exists $c = c(\varepsilon) > 0$ such that uniformly in $L \leq L(\varepsilon)$,*
$$\lim_{N\to\infty} \mu^{\varepsilon}_{N,L}\left(\frac{R \text{ has area at least}}{N^2} \geq c\right) = 1,$$
where $c(\varepsilon) \to 1$ and $L(\varepsilon) \to \infty$ as $\varepsilon \to 0$.
- *If $q > q_1$ then there exists $c = c(q) > 0$ such that*
$$\lim_{N,L\to\infty} \mu^{q}_{N,L}\left(\frac{R \text{ has area at least}}{N^2} \geq c\right) = 1,$$
where $c(q) \to 1$ as $q \to \infty$.

The first part of the above theorem is still in preparation [12], while the second part will be published soon [13].

3. Ideas of the proof

The rigidity property is a direct consequence of the following Peierls estimate:

$$\mu_{N,L}(I(\sigma) = \Gamma) \leq \delta^{w(\Gamma)}, \tag{4}$$

where $\delta = \delta(\varepsilon), \delta(q)$ is a (small) positive constant, Γ is any fixed shape of interface with *weight* $w(\Gamma) = |\Gamma| - N^2$.

To show (4) uniformly in $N, L \leq L(\varepsilon)$ in the toy model, or uniformly in N, L in its clock version, we use chessboard estimates coming from the reflection positivity property [3, 9] shared by both models. Actually, the boundary conditions we use are not fully periodic so that RP holds only for reflections with respect to vertical hyperplanes.

4. Perspectives

Eventually, we state some possible extensions of this work. First of all, the rigidity property is a good step towards the construction of Dobrushin states but

is unfortunately not sufficient. To properly obtain theses states, one has to localize the interface. This localization might be obtained by entropic repulsion considerations [11].

Then, one can try to derive similar results for other models. The application of this method to double wells or large entropy/small energy models is a work in progress [10].

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Travelling waves in atomic models for phase-transforming materials and kinetic relations

Johannes Zimmer

(joint work with Hartmut Schwetlick)

The aim is to prove the existence of travelling waves for discrete models of phase-transforming materials and derive so-called kinetic relations. The motivation is as follows. Consider the equations of motions of an elastic material,

$$u_{tt}(x) = \mathrm{Div}(\sigma(Du(x))). \tag{1}$$

Here, u is the displacement field $u\colon \Omega \to \mathbb{R}^m$, with $\Omega \subset \mathbb{R}^n$; σ is the stress tensor. Let V denote the elastic energy density, then $\sigma(F) = \frac{\partial V}{\partial F}$. For phase transitions, V

is commonly assumed to be non-convex, and σ is thus non-monotone. Equation (1) is consequently of elliptic-hyperbolic type. Our understanding of this ill-posed equation is at present very limited.

From an engineering viewpoint, this is not surprising. The ill-posed nature of Equation (1) is related to the motion of an interface between stable phases. There is no physical law describing the motion of such an interface as a function of the relevant forces.

It thus seems reasonable to study the motion of a single interface between two phases in detail. A moving interface is exposed to the so-called *configurational force* f, and we denote the velocity of the interface by c. A *kinetic relation* is a functional relationship between f and c, and will be expressed here in the form $f = f(c)$. We refer the reader to [6, 1] for more information on kinetic relations.

A number of successful models in engineering postulate a phenomenological kinetic relation to resolve the problem of being ill-posed. This obviously raises the question whether kinetic relations can be derived rigorously. A natural starting point is the atomic scale. Truskinovsky and Vainchtein obtained for such a model the existence of travelling waves [7] and derived quasicontinuum models from the microscopic picture [8]. The existence argument for waves on a bi-sided infinite chain of atom commonly relies on the so-called *causality principle for a steady-state solution* [5].

We aim to develop a simple approach for proving the existence of travelling waves in lattices, and derive kinetic relations. The precise setting is as follows. We consider a one-dimensional chain of atoms $\{q_j\}_{j\in\mathbb{Z}}$ on the real line. Neighbouring atoms are linked by a bistable spring with elastic potential V. The deformation of atom k is given by $u_k\colon \mathbb{R} \to \mathbb{R}$. The argument of the elastic potential V is the discrete strain, which is given by the difference of the deformations, $u_{k+1}(t)-u_k(t)$. The equations of motion are assumed to be governed by Newton's law. In suitable units, Newton's law reads

$$\ddot{u}_k(t) = V'(u_{k+1}(t) - u_k(t)) - V'(u_k(t) - u_{k-1}(t)) \tag{2}$$

for every $k \in \mathbb{Z}$. This is a spatially discretized, one-dimensional version of Equation (1). Since the quest for rigorous kinetic relations requires a detailed understanding of the existence of travelling waves, we switch the travelling wave formulation

$$u_k(t) = u(k - ct) \text{ for } k \in \mathbb{Z}. \tag{3}$$

Then Equation (2) becomes

$$c^2\ddot{u}(x) = V'(u(x+1) - u(x)) - V'(u(x) - u(x-1)). \tag{4}$$

We remark that this is the Euler-Lagrange function for the action functional

$$\phi(u) := \int_{\mathbb{R}} \left[\tfrac{1}{2}c^2\dot{u}(t)^2 - V(u(t+1) - u(t))\right] \mathrm{d}t.$$

To describe martensitic phase transitions, the interaction potential V is assumed to be *nonconvex*. So far, a rigorous analysis seems to be confined to special form

of V, namely a piecewise quadratic energy,

$$V(\epsilon) := \frac{1}{2}\min\{(\epsilon+1)^2, (\epsilon-1)^2\} \tag{5}$$

(here and below, we write $\epsilon := u(t+1) - u(t)$ for the discrete strain).

The aim is to investigate the existence of solutions to (4) with V given by (5). To ensure that both wells of the energy V are visited, we concentrate on heteroclinic waves with the strain distribution

$$\epsilon > 0 \text{ for } x > 0 \text{ and } \epsilon < 0 \text{ for } x < 0$$

(other ratios are possible, as discussed below). Of particular interest are subsonic waves, since kinetic relations can be shown to be relevant in this case. For V given in (5), the wave speed is 1. We develop a method to prove rigorously the existence of a solution to (4) for sufficiently large velocities below the wave speed 1. The main difficulty is that Fourier methods are not readily available, since singularities stemming from zeros of the dispersion relation have to be taken into account.

We remark that it is not hard to see that on a torus of length L, the existence of solutions with the strain distribution

$$\epsilon > 0 \text{ on } (0, \tfrac{L}{2}) \text{ and } \epsilon < 0 \text{ on } (\tfrac{L}{2}, L) \tag{6}$$

depends on the wave speed c: for some velocities c, a solution exists, while for other velocities nonexistence of a solution with strain distribution (6) can be proved.

For waves on the real line, it is possible to show that the solution satisfies the Rankine-Hugoniot conditions. Furthermore, the configurational force f can be shown to be zero, so that $f(c) = 0$ is the desired kinetic relation. A closer analysis reveals that the symmetry of the solution, imposed by the sign condition (6), leads to the vanishing configurational force. It is expected that asymmetric distributions will give rise to non-vanishing kinetic relations; the waves with asymmetric sign distribution are likely to have an interpretation as suitable limits of waves on a torus as $L \to \infty$, as in the symmetric case.

We close this report by pointing out that the interest in lattice models such as Equation (4) goes beyond the realm of phase transitions. Indeed, Equation (4) is an instance of a so-called *lattice differential equation*. Many problems, such models of crystal lattices, photonic structures, and Josephson junctions, can be described by lattice differential equations as well. There are a number of mathematical problems associated with lattice differential equations in general. A number of interesting papers [2, 3, 4] give a good insight into this field.

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