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Phasenübergänge

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Introduction by the Organisers

This workshop, as an established intention, brings together different groups working on phase transitions. Mathematicians working in statistical mechanics, and others working in PDE and continuum mechanics met with physicists with a strong experimental background.

There were many younger participants, and they specifically stated that this workshop gave them an excellent opportunity for contact with the fields different from their own.

There was a wide range of subjects presented in the talks and also in the discussion groups, with an emphasis on free energies, scalings and microstructures. The modelling aspect was very important always with the aim to get rigorous results, describe qualitative behaviour and the relationship between different classes of models in precise terms, e.g. via singular perturbation theory. This meant that the discussion of mathematical technical tools, many inspired by phase transition problems, played a large role in the workshop.

Workshop: Phasenübergänge

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Abstracts

Large deviations for the random field of gradients and their thermodynamic properties

Stefan Adams

It is a common phenomenon that at low temperature two pure thermodynamic phases spatially coexist and are separated by an interface, which is very sharp with a width of a few atomistic distances. An appropriate statistical mechanics model for the interface is the unbounded spin model; one assumes that transverse deviations from the perfectly flat interface are given through a scalar field ϕ, i.e., $\phi : \mathbb{R}^2 \to \mathbb{R}$ with $\phi \equiv 0$ corresponding to the flat interface. To have a mathematically well defined model we discretise and also generalise to arbitrary dimensions. Then $\phi : \mathbb{Z}^d \to \mathbb{R}$, and $\phi_x := \phi(x)$ is the height of the interface at site $x \in \mathbb{Z}^d$ and $(\phi_x)_{x\in\mathbb{Z}^d} \in \Omega := \mathbb{R}^{\mathbb{Z}^d}$ is called the random field of heights. Neighboring sites are connected through an elastic potential V, where we later have to restrict V to be strictly convex. In this talk we restrict to quadratic V. To each configuration ϕ we associate the formal (elastic) energy

$$H(\phi) = \frac{1}{2} \sum_{|x-y|=1} V(\phi_x - \phi_y), \tag{1}$$

which is a *massless* model due to the fact that there are no self interaction terms for single heights. The formal equilibrium measure is given by

$$Z^{-1} \exp\left(-H(\phi)\right) \prod_x d\phi_x. \tag{2}$$

In the non compact setting even the existence of thermodynamics of these interface models becomes nontrivial. These existence problems can be solved by making strong assumptions on the interactions such as superstability ([1]). Connections between equilibrium statistical mechanics and the theory of large deviations have been know for a long time ([2]). Large deviations results for the empirical field were recently given in [3, 4], where one has to consider dimensions $d \geq 3$ for the existence of limit Gibbs measures. If we fix in (2) the heights to be zero at the boundary of a box Λ, then the fluctuations grow like the volume in dimension one, respectively like the logarithmic volume in dimension two, whereas for dimensions greater equal than three they are bounded ([5]). Thus in dimension $d = 1, 2$ the infinite Gibbs measure does not exist as it is the case for $d \geq 3$.

A glance at the *massless* model (1) leads us to consider the so-called *random field of gradients* $\eta_{(x,y)} = \phi_x - \phi_y, |x - y| = 1$ for all $x, y \in \mathbb{Z}^d$. The *random field of gradients* can be seen as the image of the random field of heights under the discrete gradient mapping, i.e., as such it is a rotation free vector field. Although the scalar random field of heights is more intuitive, the *random field of gradients* seems to be more fundamental. Notice here that in dimension $d = 1$ this *random field of gradients* is an independent random walk with a linear constraint (e.g. see

[6]); this is no longer true in dimensions $d \geq 2$. In particular, we have existence of the *random field of gradients* even when the random field of heights does not exist (see [7, 8, 9]). Moreover there is a complete classification of the extremal ergodic gradient Gibbs measures in the sense that for any tilt/slope $u \in \mathbb{R}^d$ there is a unique ergodic gradient Gibbs measure, also called the Funaki-Spohn state for the given tilt/slope ([7]).

The *random field of gradients* is our central object of study. A full level-3 large deviations results will enable us to consider bounded continuous perturbations of the strictly convex elastic interaction potential V and thus to go beyond this restriction in choosing an interaction potential. Our approach will turn out to be a first step in this outlined program.

Although the *random field of gradients* turns out to be the more fundamental object of study and guarantees the existence for Gibbs measures in any dimension in the thermodynamic limit, the price one has to pay is to tackle the difficulties that the reference measure as the image measure of the product Lebesgue measure under the gradient mapping has no product structure, and that the boundary conditions do have a great influence on the Gibbs distributions in finite boxes.

As a first step we propose to consider the random field of heights but now with the so-called *gradient events*, i.e., we measure only events which are functions of the gradients. In this way we construct for any finite box $\Lambda \subset \mathbb{Z}^d$ the corresponding gradient σ-algebra and reference measure, denoted by $\mathcal{F}_\Lambda$ and λ_Λ respectively, in the following way. Via a linear mapping to a random field of height in the box $\Lambda \setminus \{x_0\}$ we can show the independence of the reference vertex $\{x_0\}$, and are able to derive some kind of sub-additivity to get the existence of the specific entropy as follows, where $\mathcal{H}_\Lambda(\mu)$ denotes the relative entropy of the measure μ with respect to the reference measure λ in the box Λ.

Theorem A. *For each translation invariant probability measure $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ and every sequence $(\Lambda_N)_{N\geq 1}$ of cubes with $|\Lambda_N| \to \infty$ as $N \to \infty$, the limit*

$$s(\mu) := -\lim_{N\to\infty} \frac{1}{|\Lambda_N|} \mathcal{H}_{\Lambda_N}(\mu),$$

exists and satisfies the equation

$$s(\mu) = \inf_{\Delta\in\mathcal{S}_\square} |\Delta|^{-1} \mathcal{H}_\Delta(\mu).$$

For each $\mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F})$ the quantity $s(\mu)$ is called the specific entropy per site (or mean entropy) of μ relative to the reference measure λ.

From this we get also the existence of the specific free energy $f(\mu)$ of a translation invariant measure μ. The surface tension $\sigma(u)$ for a given vector $u \in \mathbb{R}^d$ is given as the infimum of the specific free energy over all translation invariant measures joining the tilt/slope u. Due to the measurability of the *gradient events* we are not able to consider boundary conditions in the Hamiltonian, thus we focus

on the Gibbs distribution with so-called *free boundary condition*, i.e.

$$\gamma_\Lambda = \frac{1}{Z_\Lambda} e^{-H_\Lambda} d\lambda_\Lambda \text{ with } H_\Lambda(\phi) = \frac{1}{2} \sum_{\substack{x,y\in\Lambda \\ |x-y|=1}} (\phi_x - \phi_y)^2.$$

The empirical field is defined as $R_N(\phi) = 1/|\Lambda_N| \sum_{k\in\Lambda_N} \delta_{\theta_k \phi}$ for the centred box Λ_N with volume N^d and shift operator θ_k modulo modification with respect to the free boundary condition. Under the *free boundary* Gibbs distributions γ_{Λ_N} with strictly convex V we derive the following large deviations result for the empirical field.

Theorem B. *The measures $\gamma_{\Lambda_N} \circ R_N^{-1}$ satisfy a large deviation principle at the volume order with rate function*

$$I(\mu) := \begin{cases} f(\mu) - \inf\limits_{u\in\mathbb{R}^d} \sigma(u) \text{ ; if } \mu \in \mathcal{P}_\Theta(\Omega, \mathcal{F}) \\ \infty \text{ ; otherwise} \end{cases};$$

i.e. for any $\Gamma \subset \mathcal{P}(\Omega, \mathcal{F})$

$$\begin{aligned} \limsup_{N\to\infty} \frac{1}{|\Lambda_N|} \log \gamma_{\Lambda_N}(R_N \in \Gamma) &\leq -\inf_{\mu\in\overline{\Gamma}} I(\mu), \\ \liminf_{N\to\infty} \frac{1}{|\Lambda_N|} \log \gamma_{\Lambda_N}(R_N \in \Gamma) &\geq -\inf_{\mu\in\overset{\circ}{\Gamma}} I(\mu), \end{aligned}$$

where $\overline{\Gamma}$ and $\overset{\circ}{\Gamma}$ denote the closure and the interior with respect to the topology of local convergence.

Extensions of these results are also discussed, where attention is made to the Green function representation of the Gaussian measures. For the considered free boundary measure the Green function belongs to the simple random walk in the graph Λ killed in the reference vertex $\{x_0\}$.

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On gradient flows of some non-convex functionals of Perona-Malik type

Giovanni Bellettini
(joint work with Giorgio Fusco)

We have discussed some problems related to the gradient flow of the nonconvex functional of the gradient

$$\frac{1}{2}\int_{(0,1)} \phi(u_x)\ dx, \tag{1}$$

where $\phi(p) = \log(1+p^2)$ is the function considered by Perona-Malik in [6] in the context of image restoration. Due to the nonconvex character of the energy density ϕ, the gradient dynamic

$$u_t = \phi''(u_x)u_{xx} \tag{2}$$

associated with (1) has a forward-backward character depending on the sign of $\phi''(u_x)$. Defining a reasonable notion of weak solution to (2) (possibly in agreement with the numerical simulations) seems to be a difficult problem. Following [5] we regularize (2) by adding to F a small higher order term and consider for $0 < \epsilon < 1$ the family of functionals

$$F^\epsilon(u) := \frac{1}{2}\int_{(0,1)} \left(\epsilon^2 (u_{xx})^2 + \phi(u_x)\right)\ dx. \tag{3}$$

Numerical experiments [3] indicate the existence of three distinct time scales for the gradient dynamics associated with F^ϵ, when $\epsilon > 0$ is extremely small. In the first time scale one observes the formation of microstructures (of smoothed staircase type) where the initial datum has derivative in the nonconvex region of ϕ (unstable region). This is an interesting phenomenon which requires further theoretical investigation; at the present moment, its evidence remains an experimental fact. After the formation of microstructures, the evolution seems to be dictated by (2) in the stable region (where the initial datum has derivative in the convex region of ϕ), while the unstable region seems to remain still, at least far from its boundary points (we do not enter in the discussion on what may happen at the boundary points). In the last time scale the solution assumes a kind of staircase structure,

and one can observe a sort of evolution of the vertical heights of the steps of the stairs.

Energetical considerations lead to introduce the small parameter ν, related to ϵ by

$$\epsilon^2 = \nu^4 \phi(1/\nu) \tag{4}$$

and to define the rescaled energy

$$F_\nu(u) := \frac{F^\epsilon(u)}{\nu\phi(1/\nu)} = \frac{1}{2}\int_{(0,1)} \left[\nu^3 (u_{xx})^2 + \frac{1}{\nu\phi(1/\nu)}\phi(u_x)\right]\, dx. \tag{5}$$

Our first result is the characterization of the $\Gamma - L^1(0,1)$-limit $\mathcal{F}$ of the family $\{F_\nu\}$ as $\nu \to 0^+$. The domain of $\mathcal{F}$ consists of those $SBV(0,1)$ functions with vanishing absolutely continuous part of the distributional derivative, and

$$\mathcal{F}(u) := \sigma \sum_{x \in J_u} |u^+(x) - u^-(x)|^{\frac{1}{2}} \tag{6}$$

where J_u is the jump set of u and $\sigma > 0$ is a suitable constant.

Heuristic arguments (that deserve further investigation) suggest that the evolution of $\mathcal{F}$ should be strictly related to the solutions to the gradient flow of the functionals F_ϵ, in the third time scale. This is one of the motivations of our study of the gradient flow of (the non-convex non smooth) functional $\mathcal{F}$, and relates our results with the previous discussion on the behaviour of the ϵ-solutions approximating (2). The weak (global in time) notion we employ to define the evolution of $\mathcal{F}$ is the so-called minimizing movement [4]. Assume that the initial datum (in the domain of $\mathcal{F}$) has a finite number of jumps. It turns out that the subsequent minimizing movement $u(\tau)$ (which is piecewise constant) has the following properties. Its jump positions do not change with time. The number of jumps is nonincreasing with time: there exist $M \leq N$ singular times $0 < \tau_1 < \cdots < \tau_M$ at which there is a dropping of the number of jumps and for $\tau \geq \tau_M$, $u(\tau)$ coincides with the average of the initial datum. In the interval between two subsequent singular times, the vector of the survived jumps is determined by the ODE which expresses the gradient of $\mathcal{F}$ restricted to the finite dimensional subspace defined by the survived jumps.

Remark: The above results, obtained in collaboration with Giorgio Fusco (Univ. of L'Aquila, Italy), were announced in [1], and will appear in [2].

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Large deviations of the current in stochastic systems

Lorenzo Bertini
(joint work with A. De Sole, D. Gabrielli, G. Jona-Lasinio, C. Landim)

The basic microscopic model is given by a stochastic lattice gas with a weak external field and particle reservoirs at the boundary. More precisely, let $\Lambda \subset \mathbb{R}^d$ be a smooth domain and set $\Lambda_N = N\Lambda \cap \mathbb{Z}^d$; we consider a Markov process on the state space X^{Λ_N}, where X is a subset of $\mathbb{N}$. The number of particles at the site $x \in \Lambda_N$ is denoted by $\eta_x \in X$ and the whole configuration by $\eta \in X^{\Lambda_N}$. The dynamics of the particles is described by a continuous time Markov process on the state space X^{Λ_N} with transition rates $c_{x,y}(\eta)$ from a configuration η to the configuration obtained from η by moving a particle from x to a neighbor site y. Similar rates $c_x^{\pm}$ describe the appearance or loss of a particle at the boundary site x. We assume the rates satisfy the *local detailed balance*, see [4, II.2.6]. The reservoirs are characterized by a chemical potential γ.

We introduce the empirical measure π^N corresponding to the density as follows. For each microscopic configuration $\eta \in X^{\Lambda_N}$ and each smooth function $G : \Lambda \to \mathbb{R}$, we set $\pi^N(G) = N^{-d} \sum_{x \in \Lambda_N} G(x/N)\eta_x$ Consider a sequence of initial configurations η^N such that $\pi^N(\eta^N)$ converges weakly to some density profile ρ_0. Under diffusive scaling, the empirical density at time t converges weakly, as $N \to \infty$, to $\rho = \rho(t, u)$ which is the solution of the hydrodynamic equation [3, 4]

$$\partial_t \rho = \nabla \cdot \Big[\frac{1}{2} D(\rho) \nabla \rho - \chi(\rho) \nabla V \Big]$$

with initial condition ρ_0 and boundary condition fixed by the reservoirs. Here D is the diffusion matrix, given by the Green–Kubo formula, see [4, II.2.2], χ is the conductivity, obtained by linear response theory, see [4, II.2.5], and ∇V the external field.

We now introduce the empirical current as follows. Denote by $\mathcal{N}_t^{x,y}$ the number of particles that jumped from x to y in the macroscopic time interval $[0, t]$. Here we adopt the convention that $\mathcal{N}_t^{x,y}$ represents the number of particles created at y due to the reservoir at x if $x \notin \Lambda_N$, $y \in \Lambda_N$ and that $\mathcal{N}_t^{x,y}$ represents the number of particles that left the system at x by jumping to y if $x \in \Lambda_N$, $y \notin \Lambda_N$. The difference $J_t^{x,y} = \mathcal{N}_t^{x,y} - \mathcal{N}_t^{y,x}$ represents the total current across the bond $\{x, y\}$ in the time interval $[0, t]$. Fix a macroscopic time T and denote by $\mathcal{J}^N$ the empirical measure on $[0, T] \times \Lambda$ associated to the current. For smooth vector fields $G = (G_1, \dots, G_d)$, the integral of G with respect to $\mathcal{J}^N$ is given

by $\mathcal{J}^N(G) = N^{-(d+1)} \sum_{i=1}^d \sum_x \int_0^T G_i(t, x/N)\, dJ_t^{x,x+e_i}$, where e_i is the canonical basis and we sum over all x such that either $x \in \Lambda_N$ or $x + e_i \in \Lambda_N$. We normalized $\mathcal{J}^N$ so that it is finite as $N \to \infty$. Given a density profile ρ let us denote by $J(\rho) = -\frac{1}{2} D(\rho)\nabla\rho + \chi(\rho)\nabla V$ the current associated to ρ. If we consider an initial configuration η^N such that the empirical density $\pi^N(\eta^N)$ converges to some density profile ρ_0, then the empirical current $\mathcal{J}^N(t)$ converges, as $N \to \infty$, to $J(\rho(t))$, the current associated to the solution of the hydrodynamic equation.

We next discuss the large deviation properties of the empirical current. Fix a smooth vector field $j : [0,T] \times \Lambda \to \mathbb{R}^d$ and a sequence of configurations η^N whose empirical density converges to some profile ρ_0. Then, by the methods in [3, Ch. 10], it is possible to show that

$$\mathbb{P}^N_{\eta^N}\big(\mathcal{J}^N(t,u) \approx j(t,u)\big) \sim \exp\big\{ - N^d\, \mathcal{I}_{[0,T]}(j)\big\}$$

where the rate function is given by

$$\mathcal{I}_{[0,T]}(j) \;=\; \frac{1}{2}\int_0^T dt\, \big\langle [j - J(\rho)], \chi(\rho)^{-1}[j - J(\rho)]\big\rangle$$

in which $\rho = \rho(t,u)$ is obtained by solving the continuity equation $\partial_t\rho + \nabla\cdot j = 0$ with initial condition $\rho(0) = \rho_0$ and $\langle\cdot,\rangle$ is the inner product in $L_2(\Lambda, du)$. Of course there are compatibility conditions to be satisfied, for instance if we have chosen a j such that $\rho(t)$ becomes negative for some $t \in [0,T]$ then $\mathcal{I}_{[0,T]}(j) = +\infty$.

We next discuss how, from the time dependent large deviation principle stated above, we obtain an extension of the results of [2] for the time average of the empirical current. Given time independent profiles $\rho = \rho(u)$ and $J = J(u)$, let us introduce the functionals

$$\begin{aligned} \mathcal{U}(\rho, J) &= \frac{1}{2}\langle J - J(\rho), \chi(\rho)^{-1}[J - J(\rho)]\rangle \\ U(J) &= \inf_\rho\, \mathcal{U}(\rho, J) \end{aligned}$$

where the infimum is carried over all profiles ρ satisfying the boundary conditions and $J(\rho)$ has been defined above. When J is constant, the functional U is the one introduced in [2].

Fix some divergence free vector field $J = J(u)$ constant in time and denote by $\mathcal{A}_{T,J}$ the set of all currents j such that $T^{-1}\int_0^T dt\, j(t,u) = J(u)$. The condition of vanishing divergence on J is required by the local conservation of the number of particles. From the large deviations principle for the current we get

$$\mathbb{P}^N_{\eta^N}\Big(\frac{1}{T}\int_0^T dt\, \mathcal{J}^N(t,u) \approx J(u)\Big) \sim \exp\big\{ - N^d \inf_{j\in\mathcal{A}_{T,J}} \mathcal{I}_{[0,T]}(j)\big\}$$

Let U^{**} be the convex envelope of U, in [1] it is shown that

$$\lim_{T\to\infty} \frac{1}{T} \inf_{j\in\mathcal{A}_{T,J}} \mathcal{I}_{[0,T]}(j) = U^{**}(J)$$

we therefore have

$$\mathbb{P}^N_{\eta^N}\Big(\frac{1}{T}\int_0^T dt\ \mathcal{J}^N(t,u) \approx J(u)\Big) \sim \exp\big\{ - N^d\, T\, U^{**}(J)\big\}$$

where the logarithmic equivalence is understood by sending *first* $N \to \infty$ and *then* $T \to \infty$. This result extends [2] to $d \geq 1$, allows divergence free J, and shows that, in general, U has to replaced by its convex envelope U^{**}. An example where U is not convex is discussed in [1].

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Simulations of Diffusion Induced Segregation

Thomas Blesgen

Diffusion Induced Segregation (DIS) processes represent a particular class of segregation phenomena where the formation of (two) phases only starts after the concentration of a particular diffusor exceeds a certain threshold. The objective of the present work is to develop suitable models for the so-called chalcopyrite disease within sphalerite which is one example of DIS, compute at least approximately the actual physical free energies and make simulations closer to reality.

Model A: For $t \geq 0$ find $c = (c_1, c_2, c_3, c_4), \chi$ such that in $\Omega \subset \mathbb{R}^D$ for $t > 0$

$$0 = \operatorname{div}\Big(\sum_{j=1}^4 L_{1j}\nabla\mu_j\Big) + k^{1/b_\chi}(c_2^2 - (\kappa)^{1/b_\chi} c_1 c_3), \tag{1}$$

$$\partial_t c_i = \operatorname{div}\Big(\sum_{j=1}^4 L_{ij}\nabla\mu_j\Big) + r_i(c,\chi),\ i = 2,3,4, \tag{2}$$

$$\mu_i = \frac{\partial f}{\partial c_i}(c,\chi),\ 1 \leq i \leq 4, \tag{3}$$

$$\tau\partial_t\chi = \gamma\triangle\chi - \omega(c,\chi) \tag{4}$$

together with initial values for c and χ and Dirichlet boundary conditions for c, μ and χ. Here, c is a concentration vector, χ measures the volume fraction of the chalcopyrite phase, μ is the chemical potential. Reaction terms: $r = (r_1, \ldots, r_4)$ with $r_1 = r_3 = -\frac{1}{2}r_2 = k^{1/b_\chi}\Big(c_2^2 - \kappa^{1/b_\chi} c_1 c_3\Big)$, $r_4 = 0$. Let $\Omega_T := \Omega \times (0, T_0)$.

Model B: Let $c = (c_2, c_3, c_4)$ and drop Equation (1) and reaction terms r_i. Choose $\chi \in BV(\Omega,\ \{0,1\})$.

$$\partial_t c_i = \operatorname{div}\Big(\sum_{j=2}^{4} L_{ij}\nabla\mu_j\Big), \quad i = 2,3,4, \tag{5}$$

$$\mu_i = \chi\frac{\partial f^1}{\partial c_i}(c) + (1-\chi)\frac{\partial f^2}{\partial c_i}(c), \quad i = 2,3,4, \tag{6}$$

$$F(c,\chi) = \min_{\tilde{\chi}} F(c,\tilde{\chi}) \tag{7}$$

where

$$F(c,\chi) = \int_\Omega \gamma|\nabla\chi| + \int_\Omega (\chi f^1(c) + (1-\chi)f^2(c))$$

and f^l are the ab-initio approximations of the free energy density f_l.

Model A is an analytic model, Model B is the basis for ab-initio computations.

Theorem (Global existence result). *Under suitable growth conditions on f_l there exists a weak solution (c,μ,χ) of System (1)-(4) such that*

(i) $c \in C^{0,\frac{1}{4}}([0,T_0];\ L^2(\Omega;\mathbb{R}^4))$,
(ii) $\partial_t c \in L^2(0,T_0;\ (H_0^1(\Omega;\mathbb{R}^4))')$,
(iii) $\chi \in C^{0,\frac{1}{2}}([0,T_0];\ L^2(\Omega))$,
(iv) $\partial_t\chi \in L^2(0,T_0;\ (H_0^1(\Omega))')$,
(v) *there exists a $q>1$ such that $\ln c_j \in L^q(\Omega_T)$ for $1 \le j \le 4$,*
$\ln\chi,\ \ln(1-\chi) \in L^2(\Omega_T)$ *and in particular $0 < c_j,\ \chi < 1$ a.e.*

The solutions to Model B are in general not unique because of a non-uniqueness in χ. Uniqueness to Model A can be shown by an integration in time method.

The correct formula for the reaction terms r_i as functions of χ and c as shown above is derived by estimating the system enthalpy. This is deeply connected to the validation of the second law of thermodynamics for the model(s).

For the computation of the physically correct f_l, the harmonic approximation is used. Before the start of finite element computations, huge data basis are filled with values for $f_1(c)$ and $f_2(c)$. As in general many atomistic configurations represent the same concentration vector, each entry in the data base is the average over many atomistic computations.

For some configurations, the results of the harmonic approximation are compared with molecular dynamics simulations and it is shown that the neglection of the vibrational part of F can have a significant impact on the results.

For the computation of the elastic constants of chalcopyrite and for further validation, some quantum mechanical computations are done.

The finite element computations show best results if a stochastic term is added to the thermodynamical driving force.

Remark: As the place in this short abstract is very limited, the interested reader is referred to [1].

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Stability of interfaces and stochastic dynamics in the regime of partial wetting

Thierry Bodineau

(joint work with Dmitry Ioffe)

The phenomenological theory of equilibrated crystals dates back at least to the beginning of the century. Suppose that two different thermodynamic phases (say a crystal and its vapor) coexist at a certain temperature T. Assuming that the whole system is in equilibrium, in particular that the volume v of the crystalline phase is well defined, what could be said about the region this phase occupies? The phase regions are quantified by the value of the free energy of the crystal-vapor interface, or by the total surface tension between the crystal and the vapor. Equilibrium shapes correspond, in this way, to the regions of minimal interfacial energy and therefore lead to an isoperimetric-type problem known as the Wulff isoperimetric problem.

A lot of efforts have been devoted to the understanding of the phase coexistence mechanisms starting from a particle system with microscopic interactions. In particular the Wulff construction for the two-dimensional Ising model is by now very well understood (see for example [9, 16, 12, 13, 14, 17, 3]). In dimension three and more, a different approach was devised which provides a weaker characterization of phase segregation (see for example [1, 2, 18, 7, 8, 4, 5]). In particular the interface structure in higher dimension is far from being understood.

There is also a strong interplay between the equilibrium and dynamical properties of particle systems. We refer to the lecture notes by Martinelli [15] and Guionnet, Zegarlinski [11] for a survey on this issue. In the phase transition regime, the slow relaxation of particle systems is due to the slow motion of the interfaces. The slowdown of the dynamics can be related to the behavior of the spectral gap of the dynamics as number of spins in the system increases. On the other hand, the spectral gap can be obtained in terms of a variational formula which involves only the equilibrium Gibbs measure.

The topic of this talk is to explain how the equilibrium results on phase coexistence in dimension larger or equal to three can be used to derive some properties of the Glauber dynamics. In particular, we show that the spectral gap of the Ising model in the domain $\{-N,\dots,N\}^d$ with free boundary conditions vanishes like $\exp(-cN^{d-1})$. This extends to higher dimensions previous results by Martinelli [15] on the spectral gap of the two-dimensional Glauber dynamics. This result is related to the stability property with respect to the Hausdorff distance of a coarse grained representation of the interface between the two pure phases of the Ising model. Thus, a key ingredient to characterize the spectral gap was to derive more

precise controls on the interface structure. We also prove that the metastable behavior can be understood in terms of the wetting transition [10, 6]. This implies that the metastability threshold depends only on equilibrium quantities.

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Nucleation in Kawasaki dynamics

Anton Bovier

(joint work with F.R. Nardi, W.Th.F. den Hollander)

We study the metastable behavior of the lattice gas in two and three dimensions subject to Kawasaki dynamics at low temperature and low density. Particles live on a finite box, hop between nearest-neighbor sites, have an attractive interaction

when they sit next to each other, and are created, respectively, annihilated at the boundary of the box in a way that reflects an infinite gas reservoir. We are interested in how the system *nucleates*, i.e., how it reaches a full box when it starts from an empty box. Our goal is to improve on earlier work by combining a detailed analysis of the energy landscape for the dynamics with the potential theoretic approach to metastability that was developed in Bovier, Eckhoff, Gayrard, and Klein [3] and further exposed in Bovier [1].

Our main theorems sharpen those obtained by den Hollander, Olivieri, and Scoppola [7] in two dimensions and by den Hollander, Nardi, Olivieri, and Scoppola [6] in three dimensions. In particular, in two dimensions we identify the full geometry of the set of critical droplets, compute the average nucleation time up to a multiplicative factor that tends to one in the limit of low temperature and low density, express the proportionality constant in terms of certain capacities associated with simple random walk, and compute the asymptotic behavior of this constant as the system size tends to infinity. In three dimensions, we obtain similar results but with less control over the geometry and the constant.

Our results are comparable with those derived by Bovier and Manzo [5] for the Ising model on a finite box in two and three dimensions with periodic boundary conditions subject to Glauber dynamics at low temperature. This work sharpened earlier results by Neves and Schonmann [9] in two dimensions and by Ben Arous and Cerf [2] in three dimensions.

Kawasaki differs from Glauber in that it is a *conservative dynamics*: particles are conserved in the interior of the box. This creates a complication in controlling the growing and the shrinking of droplets, because particles have to travel between the droplet and the boundary of the box. Moreover, it turns out that in the metastable regime *particles move along the border of a droplet more rapidly than they arrive from the boundary of the box*. This leads to a shape of the critical droplet that is more complicated than the one for Ising spins under Glauber dynamics. This complexity needs to be handled in order to obtain the sharp asymptotics. For a critical comparison of Glauber and Kawasaki we refer to den Hollander [8]. Nonetheless, the basic approach of [3] can be made to work rather nicely and provides very satisfactory results. In particular, it allows to represent the mean nucleation time up to multiplicative errors that tend to one as $\beta \uparrow \infty$ as the usual Kramer exponential factor $e^{\beta\Gamma}$ times a volume dependent prefactor of the form $K \ln|\text{Ł}|/|\Lambda|$ (in $d = 2$, resp., $K/|\Lambda|$, where the constants K can be interpretated in terms of the local geometry of the critical droplets and a capacity related to simple random walk. In $d = 2$, the constant can be computed explicitely in the limit of volumes.

Details can be found in [4].

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A superfluidity theory for the non-dilute Bose gas

Jean-Bernard Bru
(joint work with S. Adams)

1. Let a homogeneous gas of n spinless bosons with mass m be enclosed in a cubic box $\Lambda \subset \mathbb{R}^3$ of volume $V \equiv |\Lambda| = L^3$. The one-particle energy spectrum is then $\varepsilon_k \equiv \hbar^2 k^2/2m$ and, using periodic boundary conditions, $\Lambda^* \equiv \left(\frac{2\pi}{L}\mathbb{Z}\right)^3 \subset \mathbb{R}^3$ is the set of wave vectors.
The considered system is non-dilute and with interactions defined via a (real) two-body soft potential $\varphi(x) = \varphi(\|x\|) \in L^1\left(\mathbb{R}^3\right)$. Note that its (real) Fourier transformation satisfies: $\lambda_0 > 0$ and $0 \leq \lambda_k = \lambda_{-k} \leq \lambda_0$ for $k \in \mathbb{R}^3$. These conditions may be relaxed in our final model, see [1]. Let $\{a_k^*, a_k\}$ be the usual boson creation/annihilation operators in the one-particle state $\psi_k(x) = V^{-\frac{1}{2}} e^{ikx}$, $k \in \Lambda^*$, $x \in \Lambda$, acting on the usual boson Fock space.

2. It is clear that, in various respects, the Bogoliubov theory [2] is inappropriate as the model of superfluidity for non-dilute systems as liquid Helium 4 [3, 4, 5]. To get interesting results on non-dilute gases for any temperatures and densities, we follow the method mainly explained in [5]. Indeed, the most important terms in the corresponding Hamiltonian with the full interaction should be those in which at least two operators a_0^*, a_0 appear, as Bogoliubov originally pointed it out [2]. Actually, this theory and the Bogoliubov one have behind them the fundamental hypothesis originally given by Fritz London [6] about existence in the system of a Bose condensation in the zero-mode. However, in contrast with the Bogoliubov theory, the truncation is here *partial*, in the sense that we do not take into account the Mean-Field interaction since it is a constant in the canonical ensemble.
Within the framework of the canonical ensemble, this procedure then implies the

new Hamiltonian:

$$H_\Lambda \equiv \sum_{k\in\Lambda^*} \varepsilon_k a_k^* a_k + \frac{1}{2V} \sum_{k\in\Lambda^*\setminus\{0\}} \lambda_k a_0^* a_0 \left(a_k^* a_k + a_{-k}^* a_{-k}\right) + \frac{1}{2V} \sum_{k\in\Lambda^*\setminus\{0\}} \lambda_k \left(a_k^* a_{-k}^* a_0^2 + {a_0^*}^2 a_k a_{-k}\right).$$

This Bose gas is quartic, non-diagonal, and far from the ideal or dilute gas. It is coherently solved in the canonical ensemble [1].

3. Actually, at any temperatures $\mathrm{T} \geq 0$ below a critical temperature T_c, the corresponding Bose gas is a mixture of particles inside and outside the Bose condensate, i.e., there is a depletion of the Bose condensate. Even at zero-temperature, our interpretation is that two Bose subsystems coexist: the Bose condensate and a second system, denoted here as the *Bogoliubov system*. This comes from a *non-diagonal* interaction, which, in particular, implies an effective attraction between bosons in the zero kinetic energy state, i.e. in the Bose condensate. In contrast with the (conventional) Bose-Einstein condensation, these bosons pair up via the Bogoliubov system to form "Cooper-type pairs" or interacting (virtual) pair of particles. This Bose condensation constituted by Cooper-type pairs is non-conventional, i.e. turned on by the Bose distribution but completely transformed by interaction phenomena.

The coherency due to the presence of the Bose condensation is not enough to make the Perfect Bose Gas superfluid, see discussions in [2]. The spectrum of elementary excitations has to be collective. In this theory, the particles outside the Bose condensate (*the Bogoliubov system*) follow a *new* distribution, different from the Bose distribution, which we call the *Bogoliubov distribution.* The Bogoliubov system coming from the depletion of the Bose condensate is a model of "quasi-particles" or linked pair of particles with the Landau-type excitation spectrum. Therefore, following Landau's criterion of superfluidity [7] it is a *superfluid* gas. The corresponding "quasi-particles" are created from two particles respectively of momenta p and $-p$ ($p \neq 0$) through the Bose condensate ($p = 0$) combined with phenomena of interaction.

Note that we can also distinguish a particle system I inside the Bogoliubov system which density explicitly depends on the temperature T and the remaining system II together with the Bose condensate. In fact, it is conjectured in [1] that the system I is the normal liquid, which is the carrier of the total entropy of the system. The system II is then the superfluid liquid (i.e. with no viscosity).

The theoretical critical temperature where the Landau-type excitation spectrum holds equals $\mathrm{T}_c \approx 3.14$ K. For the liquid ^{4}He, the superfluid liquid already disappears at $\mathrm{T}_\lambda = 2.17$ K, but the Henshaw-Woods spectrum[1][8] does *not* change drastically when the temperature crosses T_λ: there is a temperature $\widetilde{\mathrm{T}}_\lambda$ where the Landau-type excitation spectrum persists for $\mathrm{T}_\lambda < \mathrm{T} < \widetilde{\mathrm{T}}_\lambda$.

[1]measure of the excitations spectrum in liquid ^{4}He by a weak-inelastic neutron scattering (1961).

4. Before finishing this summary, we recall that this analysis is based on a truncation of the full interacting Bose gas in the canonical ensemble. This *unique* truncation hypothesis is still not proven, but it is shown [1] that the theory is, at least, self-consistent. Note that the proofs are technically based on three papers [9, 10]. We use the "superstabilization" method [9] to analyze the corresponding model in the canonical ensemble from the grand-canonical one. This study is possible since the exact solution of the (non-diagonal) AVZ-Hamiltonian [3], also called the superstable Bogoliubov Hamiltonian, is found in the grand-canonical ensemble by the paper [10].

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Graded cluster expansion for renormalized systems

Emilio N.M. Cirillo
(joint work with L. Bertini, E. Olivieri)

We have analyzed the Block Averaging Transformation applied to the two–dimensional Ising model in the uniqueness region. We studied the Gibbs property of the renormalized measure and the convergence of renormalized potential under iteration of the map. It turns out that for any temperature T higher than the critical one T_c the renormalized measure is strongly Gibbsian [1], whereas for $T < T_c$ we have only weak Gibbsianity [4]. We note that in this region it has been proven that, for a peculiar choice of the parameters, the renormalized measure is not gibbsian [5]. Accordingly, we have convergence of the renormalized potential in a strong sense for $T > T_c$ and in a weak sense for $T < T_c$. Since we are arbitrarily close to the coexistence region we have a diverging characteristic length of the system: the correlation length or the critical length for metastability, or both. Thus, to perturbatively treat the problem we use a scale–adapted expansion [7, 8]. The more delicate case is $T < T_c$ where we have a situation similar to that of a

disordered system in the presence of a Griffiths' singularity namely, the lattice is made of a good region, in which the system is weakly coupled, and a bad region where it is not. In this case we use a graded cluster expansion whose minimal scale length is diverging when approaching the coexistence line.

We study the problem in the context of systems with no random disorder in the interactions; however, we suppose deterministically possible to analyze the bad interactions on suitable increasing scale lenghts [3]. We treat iteratively the regions of increasing badness and prove convergence of the expansion on the basis of suitable assumptions on the potential in the good region and sufficient "sparseness" of bad regions.

The assumption that the system is weakly coupled on the the good part of the lattice is formalized as follows. Let Δ be a finite subset of the good region and $Z_\Delta(\sigma)$ be the partition function in Δ with boundary condition σ. We assume

$$\log Z_\Delta(\sigma) = \sum_{X \cap \Delta \neq \emptyset} V_{X,\Delta}(\sigma)$$

where the effective potential $V_{X,\Delta}$ have a suitable decay property w.r.t. X uniformly in Δ and σ.

The expression above can be obtained via cluster expansion in the weak coupling (high temperature and/or small activity) region but it also holds in the more general situation of the scale–adapted cluster expansion discussed before. In the latter case it holds provided the volume Δ is a disjoint union of cubes whose side length equals the scale L of the expansion.

The main result of the graded cluster expansion [3], inspired by the techniques in [6], concerns an expression, similar to the one above, of the logarithm of the partition function on a generic finite subset of the whole lattice, possibly intersecting its bad region. Its characteristic feature, with respect to a usual low activity expansion, is that here polymers are geometrical objects living on arbitrarily large scale. More precisely, for each finite subset of the lattice Λ and boundary condition σ we have the following totally convergent expansion

$$\log Z_\Lambda(\sigma) = \sum_{X \cap \Lambda \neq \emptyset} [\Psi_{X,\Lambda}(\sigma) + \Phi_{X,\Lambda}(\sigma)]$$

where $\Psi_{X,\Lambda}$ and $\Phi_{X,\Lambda}$ depend on σ inside $X \cap \Lambda^{\mathrm{c}}$. The Ψ's are short range in the sense that for each site x of the lattice there exists a positive r_x such that $\Psi_{X,\Lambda} = 0$ if the diameter of X exceeds r_x. On the other hand the Φ's are long range but uniformly bounded in the sense that there exists a positive c such that

$$\sup_x \sum_{X \ni x} \sup_\sigma |\Phi_{X,\Lambda}(\sigma)| \leq c$$

As a final remark it is worth noting that by using the proven expansion and results in [2] it is possible to deduce the exponential decay of correlations of local functions.

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Two-dimensional structures in ferroelastic domain walls

Sergio Conti

The structure of ferroelastic materials can be studied within the framework of continuum mechanics via models of the type

$$E[u] = \int_\Omega W_b(\nabla u) + \varepsilon^2 |\nabla^2 u|^2 dx + \int_{\partial\Omega} W_s(\nabla u) d\mathcal{H}^{n-1}$$

where $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}^n$, $W_b : \mathbb{R}^{n\times n} \to \mathbb{R}$ is a double-well potential (bulk energy), and W_s represents the surface energy, i.e., the correction to W_b which is needed close to free boundaries. For small ε one expects $E[u]$ to reduce to a sharp-interface model, whose minimizers depend only on one variable (and this can indeed be proven if $n = 2$, see [3]). We address deviations from the one-dimensional minimizers of the limiting sharp-interface model which arise for small but finite ε. We assume all over that $n = 2$ and use geometrically linear elasticity for simplicity; most results can be extended to nonlinear elasticity and $n = 3$ without qualitative changes.

We start by studying the surface structure of a domain wall, namely, the modifications that occur in the vicinity of a free boundary. For definiteness, we assume that

$$W(\nabla u) = \frac{1}{2} C_{11} \left(u_{x,x}^2 + u_{y,y}^2\right) + C_{12} u_{x,x} u_{y,y} + \frac{1}{8} C_{44} \left(e^2 - 1\right)^2$$

where $e = u_{x,y} + u_{y,x}$ is the ferroelastic order parameter. The surface energy term takes the form

$$W_s(\nabla u) = \frac{1}{2} \gamma\varepsilon C_{44} (u_{x,y} + u_{y,x})^2 \,.$$

This expression, first used in [2], is heuristically motivated by the experimentally known fact that the order parameter is typically reduced in the presence of free boundaries.

In a first work in collaboration with E. Salje [2] a similar model was studied by means of an expansion on a finite set of basis functions, which is feasible if the phase distribution is a priori known. This is appropriate for example if the domain wall is orthogonal to the free surface. Numerical results showed a double peak in the surface structure of the order parameter, which is related to the chemical reactivity of the system and hence can be compared to experiments on selective doping. The numerical results turned out to be in good agreement with atomistic computations by Novak and Salje [7, 8]

In subsequent work in collaboration with U. Weikard [4] the model above was studied with adaptive finite elements, based on the visualization library GRAPE developed in the SFB 256 in Bonn. This permits to study the general case, where the wall is not orthogonal to the free surface and the phase distribution is a priori unknown. Our results show a significant bending of the domain wall towards the surface. We understand this by means of a simple one-dimensional approximate model. The model is based on the interplay between the elastic energy generated by the incompatibility and the line tension of the interface, and gives results in good agreement with the finite element simulations.

In a second part of this talk possible complex structures in domain walls away from interfaces have been presented. In particular, in joint work with B. Schweizer [3] it was shown that for bulk energies of the form

$$W_b(\nabla u) = \big(1 - (u_{x,y} + u_{y,x} - 1)^2 + \alpha u_{x,x} u_{y,y}\big)^2 + u_{x,x}^2 + u_{y,y}^2\,,$$

depending on the values of the parameter α, the one-dimensional profile is not optimal, and structures tangential to the interface necessarily develop. Finite-element simulations based on the same code discussed above show that a periodic structure develops tangential to the domain wall [5], which is reminiscent of cross-tie walls in ferromagnetic thin films [6, 1].

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Tunnelling in non local evolution equations

Anna De Masi
(joint work with G. Bellettini and E. Presutti)

Tunnelling is a phenomenon which describes transitions between two stable states of a system. The origin of the phenomenon is ascribed to stochastic fluctuations which are either due to "intrinsic randomness" in the system, or to "random external forces" or to both. In all cases, one is interested in the waiting time for the tunnelling to take place, the nature of the forces which drive the tunnelling and the specific pattern of the tunnelling event.

As a mathematical model of the phenomenon, we consider a non local evolution equation which has been introduced in connection with the analysis of Ising systems with Kac potentials, [3]. Our setting is one dimensional, and the free energy associated to this model in the interval $[-L, L]$, $L > 1$, is:

$$\mathcal{F}_L(m) = \int_{-L}^{L} \phi_\beta(m)dx + \frac{1}{4}\int_{-L}^{L}\int_{-L}^{L} J^{\text{neum}}(x,y)(m(x)-m(y))^2 dxdy, \tag{1}$$

where, given $J(x,y)$, $(x,y) \in \mathbb{R}\times\mathbb{R}$, a smooth, symmetric, translational invariant probability kernel supported by $|y-x| \le 1$, by J^{neum} we denote the kernel with reflections at $\pm L$. Furthermore

$$\phi_\beta(m) = \tilde{\phi}_\beta(m) - \min_{|s|\le 1}\tilde{\phi}_\beta(s), \quad \tilde{\phi}_\beta(m) = -\frac{m^2}{2} - \frac{1}{\beta}S(m) \tag{2}$$

$$S(m) = -\frac{1-m}{2}\log\frac{1-m}{2} - \frac{1+m}{2}\log\frac{1+m}{2} \tag{3}$$

The evolution equation for $u = u(x,t)$, $|x| \le L$, $L > 1$, $t \ge 0$ is the gradient flow, namely, (u_t below is the t-derivative of u):

$$u_t = f_L(u), \qquad f_L(u) = -\frac{\delta\mathcal{F}_L(u)}{\delta u} \tag{4}$$

Neumann boundary conditions simplify the analysis, as, for instance, the stationary, space homogeneous solutions of (4) turn out to be independent of L. These are denoted by $\pm m_\beta$, with $m_\beta > 0$ solving the mean field equation

$$m_\beta = \tanh\{\beta m_\beta\}, \quad (\beta > 1) \tag{5}$$

It can be seen that $\pm m_\beta$ are locally stable, so that they play here the role of pure phases and the tunnelling events which occur within a time $\tau > 0$ are then represented by the set $\mathcal{U}_\tau^{\pm}$ of orbits $u(\cdot,t)$, $t \in [0,\tau]$ such that $u(\cdot,0) = -m_\beta$, $u(\cdot,\tau) = m_\beta$. Due to the stationarity of $\pm m_\beta$, no element in $\mathcal{U}_\tau^{\pm}$ can satisfy (4) and therefore other forces must enter into the game. Their choice can be related to a Lagrangian action in the following way. Call $b = b(x,t)$, $|x| \le L$, $0 \le t \le \tau$, an "external force", and consider the corresponding evolution equation

$$u_t = f_L(u) + b \tag{6}$$

We are of course only interested in forces b able to produce orbits in $\mathcal{U}_\tau^\pm$. To select among them we introduce an action functional

$$I_\tau(u) = \frac{1}{4}\int_0^\tau \int_{-L}^L b^2\, dx\, dt \equiv \frac{1}{4}\int_0^\tau \int_{-L}^L \big(u_t - f_L(u(\cdot,t))\big)^2\, dx\, dt \tag{7}$$

which is interpreted as "the cost" of the force field b which produces the orbit u. In other words, $I_\tau(u)$ is the penalty assigned to the orbit u; thinking of b as an electric field, (7) is the dissipation due to a constant resistivity, whose value in (7) is set equal to $1/4$.

In the above setting, it looks natural to ascribe the actual tunnelling event to the force field which has the minimal cost: this leads to the variational problem

$$P^\pm := \inf_{\tau>0} \inf_{u\in\mathcal{U}_\tau^\pm} I_\tau(u) \tag{8}$$

The variational problem with $\tau > 0$ fixed, is exactly the Euler Lagrange variational problem with Lagrangian $\mathcal{L}(u, u_t) = (u_t - f_L(u))^2/4$. The corresponding Euler Lagrange equations are,

$$b_t = -bf_L'(u) \tag{9}$$

which we may regard as an equation on b with u determined by b through the equation (6). (9) is then the equation for the optimal force needed for tunnelling. In statistical mechanics, the forces b are random and their probability is a datum of the problem: thus one knows, in principle, the probability of any possible force field b in (6) and in particular of those which give rise to a tunnelling. These probabilities are expected to be very small, exponentially small with an exponent proportional to $-\epsilon^{-d}$ (d the space dimension, here $d = 1$), $\epsilon > 0$ a small parameter which represents the ratio between microscopic and macroscopic lengths. The proportionality coefficient is called the "rate function of large deviation" and we interpret our $I_\tau(u)$ as such a rate function. Thus we are supposing that the probability of observing u goes like $\exp\{-\epsilon^{-d} I_\tau(u)\}$ and since the time to wait before observing an event is proportional to the inverse of its probability, the expected time T for tunnelling, will go like $\exp\{\epsilon^{-d} P^\pm\}$. Thus the main interest in statistical mechanics is to estimate the proportionality coefficient $P^\pm$, which we do in following theorem.

Theorem. *For any L large enough,*

$$\inf_{\tau>0} \inf_{u\in\mathcal{U}_\tau} I_\tau(u) = \mathcal{F}_L(\hat m_L) \tag{10}$$

$\hat m_L$ is an antisymmetric function stationary solution of (4)*, namely it solves*

$$\hat m_L(x) = \tanh\{\beta J^{\mathrm{neum}} * \hat m_L(x)\}, \quad |x| \le L \tag{11}$$

The next problem is to understand how the tunnelling proceeds once it starts and this is described by the minimizing sequences which realize $P^\pm$. This problem in our context has a quite complete and detailed answer. In fact, a much more refined analysis of (4), shows that there are two invariant, one dimensional manifolds $\mathcal{M}^\pm$, connecting $\hat m_L$ to $-m_\beta$ and to m_β, see (5). This statement has been

proved in [2], see also [4], for a dynamics which is closely related to the one we are considering, and we show that the results extend to the present case.

We prove that all the minimizing sequence are very similar to each other, following (4) in some parts of the tunnelling orbit and its time reversal, in other parts. Roughly speaking, the solution to (8) is given by an orbit which is made by patching together the time reversed of $v^{(-)} \in \mathcal{M}^-$ and $v^{(+)} \in \mathcal{M}^+$. While it is well established that a minimizing sequence can be obtained by following the reversed flow on the invariant manifolds, our result completes the picture by saying that "this is in fact the only possible way", as any other pattern would lead to a larger penalty. The time for the tunnelling, once it starts, is dictated by the flow along the invariant manifolds, except for the motion close to its endpoints, which can be reached only after an infinite time, if moving all the way along the invariant manifolds. To keep the time τ finite, we then need to depart from the manifolds, with "shortcuts" close to the endpoints.

The relation between variational problems and large deviations is well established, see the classical reference text by Freidlin and Wentzel, [6]. The application of the theory to tunnelling in the spirit outlined above has been first and beautifully carried out by Faris and Jona-Lasinio, [5], in the context of the stochastic Allen Cahn equation $u_t = u_{xx} + \phi(u) + \sqrt{\epsilon} b$ for a particular choice of force ϕ, with b a standard white noise in space-time and with Dirichlet boundary conditions at $\pm L$. The rate function in such cases has a structure similar to (7) and we in fact use many of the ideas contained in [5]. Their adaptation to (4) is from one side simpler, because we only look at the variational problem and avoid all questions concerning probabilities, but, on the other side, it brings in new difficulties, as we miss a characterization of the stationary solutions of the deterministic problem (i.e. without b) which are instead easy in the case $u_{xx} + \phi(u) = 0$.

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Large-time behavior for Hamilton-Jacobi equations forced by additive noise

Nicolas Dirr
(joint work with P.E. Souganidis)

We are interested in the long-time behavior of solutions to equations of the form

$$\mathrm{d}u - (\mathrm{tr}A(x)D^2u - H(Du,x))\mathrm{d}t + \mathrm{d}W(x,t) = 0 \quad \text{in } \mathbb{R}^n \times (0,\infty)\ , \tag{1}$$

where both $A(x)$ and $H(x,p)$ are Lipschitz-continuous and periodic with respect to x. Moreover, we assume that there exists a periodic, Lipschitz-continuous matrix-valued function σ such that $A = \sigma\sigma^T$.

The random noise has the form $\mathrm{d}W(x,t) = \sum_{i=1}^{M} F_i(x)\mathrm{d}W_i(t)$, where the W_i are Brownian motions and $F_i \in C^2(\mathbb{R}^n)$ is periodic in x. We use the property that the Brownian motion has almost surely continuous sample path, independent increments, and that the event $\{\sup_{t\in[0,l]} |W(t) - W(0)| < \epsilon\ \}$ has positive probability for all $\epsilon > 0$. In the view of this, our analysis extends to other types of random forcing. Moreover, using discontinuous viscosity solutions, it is possible to extend our analysis to equations driven by certain jump processes, like, for example, kicking force.

Our results hold for all initial data and initial times and for all realizations of the noise in a set of full measure.

We denote by $C(\mathbb{T})$ the space of periodic in x continuous real valued functions on $[0,1]^n$. For $w \in C(\mathbb{T})$, we write $|||w||| = \inf_c \|w - c\|$. Moreover we denote by $S^{W,A}(t,s)(u)$ the solution of (1) starting with initial datum u at s. As the semigroup commmutes with adding a constant to u, the norm introduced above is the appropriate notion of convergence.

$S^{0,A}$ denotes the solution of the deterministic version of (1), i.e. the solution of the equation

$$v_t - \mathrm{tr}A(x)D^2u + H(Du,x) = 0 \quad \text{in} \quad \mathbb{R}^n \times (0,\infty)\ . \tag{2}$$

Our main result can be summarized in the following way. Let $H(x,p)$ be bounded from below, superlinear in p, and such that there exists an increasing function Φ such that, for some $\delta > 0$, $\Phi(r)r^{-(1+\delta)} \to \infty$ as $r \to \infty$, and

$$p \cdot D_pH(p,x) - H(p,x) \geq \Phi(|p|)$$

for all (p,x) with $|p|$ sufficiently large. This is some form of asymptotic convexity of the level sets of H. Moreover assume that (2) has a unique up to constants periodic in space and global in time attracting solution, i.e. there exist a unique $\lambda \in \mathbb{R}$ and a unique up to constants $U \in C(\mathbb{T})$, which depends on A and H, such that, for all $v \in C(\mathbb{T})$ and $t_0 \in \mathbb{R}$, there exists $c \in \mathbb{R}$ such that

$$\lim_{N\to\infty} \sup_{x\in\mathbb{T}} \left| S^{0,A}(t_0+N,t_0)(v) - (U+c) - \lambda N \right| = 0.$$

Then the stochastic Hamilton-Jacobi equation (1) also has a unique up to constants periodic in x and global in time attracting solution, i.e. there exists a unique

up to constants solution $u_{inv}(\cdot,\cdot,\omega)$ of (1) such that for any $v \in C(\mathbb{T})$, $s \in \mathbb{R}$,

$$\lim_{t\to\infty} |||u^A_{inv}(\cdot,t,\omega) - S^{W,A}(t,s)(v)(\cdot)||| = 0 \ .$$

As $A \to 0$, these attracting solutions converge to attracting solutions of the first-order equation. Indeed, assume that $A = \epsilon\tilde{A}$ is uniformly elliptic. If $u^\epsilon_{inv}(\cdot,\cdot,\omega)$ and ${u_{inv}}^0(\cdot,\cdot,\omega)$ are the attracting solutions of (1) corresponding to $\epsilon > 0$ and $\epsilon = 0$ respectively, then, for any $[a,b]$,

$$\lim_{t\to\infty} \sup_{[a,b]} |||u^\epsilon_{inv}(\cdot,t,\omega) - u^0_{inv}(\cdot,t,\omega)||| = 0 \ .$$

The problem under consideration here is a "toy" example for far more complex models in, for example, fluid mechanics (stochastically forced Navier-Stokes equation) and phase transitions and growth processes (the so-called KPZ (Kadar-Parisi-Zhang) equation).

Another example to which our results apply is the stochastic Burger's equation with additive noise, because if u solves the stochastic Hamilton-Jacobi equation, then $v = u_x$ solves Burger's equation. The unique up to constants random attractor of the Hamilton-Jacobi equation yields a unique invariant measure for Burger's equation.

Invariant measures of the stochastic Burgers equation and other closely related equations have been the object of extensive study. We refer to E, Khanin, Mazel and Sinai [4], Iturriaga and Khanin [7], Gomes, Iturriaga, Khanin and Padilla [6] for Burger's equation.

The large-time behavior of solutions (2) depends strongly on whether $A \equiv 0$ or uniformly elliptic, while very little is known in the degenerate case. When $A = 0$ and H is periodic in time, it was shown by Barles and Souganidis [1] (see also Fathi and Mather [5]) that there are no global attracting solutions. Phenomena like period doubling can occur. Our result shows that this cannot happen if the time dependence of the coefficients is very irregular, like a path of the Brownian motion.

The proofs in our paper are based on general arguments from the theory of viscosity solutions. This allows to consider general Hamiltonians H and matrices A. In view of the generality of our assumptions, this note extends previous works of Iturriaga and Khanin [7], E, Khanin, Mazel and Sinai [4] and Gomes, Iturriaga, Khanin and Padilla [6], which consider strictly convex Hamiltonians. For such Hamiltonians the solution of (1) can be expressed as the value function of a control problem. The asymptotic behavior of the solutions then reduces to the study of the corresponding controlled stochastic and ordinary differential equations.

For the "correct" interpretation of solutions of (1) we use the ideas of the theory of fully nonlinear stochastic pde developed by Lions and Souganidis in [9], [10] and [11], which applies to more general equations. This allows to consider pathwise solutions which can be expressed, up to a simple transformation, as solutions of a pde with random coefficients. For this, we need the equation

$$v_t - trA(x)D^2v + H(x, Dv + DW(x,t,t_0)) = \mathrm{tr}A(x)D^2W(x,t,t_0). \tag{3}$$

A function u is a viscosity solution of (1) on $\mathbb{T} \times [a, b]$, if the function

$$v(x, t, \omega) = u(x, t, \omega) - \int_a^t \mathrm{d}W(x, s)$$

is a viscosity solution of (3) for $a < t < b$.

The crucial step in our proof is to show that, after a time of order one, the solutions of (1) become Lipschitz continuous with respect to x with a Lipschitz constant which depends on the realization of the noise, but is independent of the initial datum.

When the Hamiltonian is super-linear but not sub-quadratic and the equation is of second order, the estimate is delicate. In this case we have to obtain the Lipschitz bound without using a-priori L^∞-bounds for nonnegative solutions, which may not exist.

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On Phase Diagrams and Diffusional Problems in the Presence of Surface Tension and Multiaxial Stresses

Wolfgang Dreyer
(joint work with Frank Duderstadt)

1. Introduction

Phase transitions in solids are usually strongly influenced by surface tension and multiaxial stresses which give rise to nonzero stress deviators. A case at hand regards the nucleation of liquid droplets in semi-insulating GaAs where deviatoric stresses result from the liquid/solid volume misfit. In turn, the nucleation barrier is determined by surface tension and the stress deviator at the interface. The latter quantity may reduce the barrier to zero.

The talk adresses two problems: 1. The calculation of phase diagrams relies on the determination of the extrema of the free energy of the considered system. The usual standard phase diagrams from the existing literature do not take into account surface tension and deviatoric stresses, and they contain exclusively the minima of the free energy. We calculate non-standard phase diagrams for the problem at hand, where the liquid phase consists of small droplets so that surface tension and deviatoric stresses become important phenomena. Furthermore we include the maxima of the free energy, because these refer to the size of critical droplets. 2. The evolution of liquid droplets in semi-insulating GaAs is due to diffusional processes in the vicinity of the droplet. The diffusion flux results from a competition of chemical and mechanical driving forces, which may imply various unexpected conditions whereupon a droplet may grow or shrink. However, due to lack of space, we only consider the first problem in this report.

The quantity of central importance for the description of all these phenomena is the chemical potential. Its calculation in the presence of mechanical stresses is one of the subjects of this study. We determine the chemical potential in the framework of the St.Venant–Kirchhoff law, which gives an appropriate stress/strain relation for many solids in the small strain regime, Subtle problems regarding the chemical potential appear in the limit where the St.Venant–Kirchhoff law is approximated by the well known Hooke law.

2. Basic variables

The thermodynamic description of semi-insulating GaAs relies on three fcc sublattices, denoted by α, β, γ, with equal densities of lattice sites. There are three different species on the sublattices, viz. Ga, As and vacancies, V, and when they are found on different sublattices, the species are considered as different constituents. We indicate this fact by the notation, Ga_α, As_α, V_α, As_β, V_β, As_γ, V_γ, and we have thus 7 constituents with mole densities n_a, $a \in \{Ga_\alpha, As_\alpha, V_\alpha, As_\beta, V_\beta, As_\gamma, V_\gamma\}$. These variables are supplemented by the displacement, u^i, so that there are 7+3

variables in the solid phase. The variables in the liquid phase are the 2 mole densities n_{Ga_L} and n_{As_L}. The details of the constitution of GaAs can be found in [2].

3. Description of deformation

Let be $X = (X^i) = (X^1, X^2, X^3)$ the location of a material point of the solid in the reference state, and $x = (x^i) = (x^1, x^2, x^3)$ its location at time t. The function $x = (\chi^i(t, X))$ gives the motion of X and $U^i(t, X) = \chi^i(t, X) - X^i$ is the displacement field. The deformation gradient is defined by $F^{ij} = \partial\chi^i(t, X)/\partial X^j$, $J = \det(F^{ij})$ is the Jacobian and the deformation is described by the right Cauchy Green tensor $C^{ij} = F^{mi}F^{mj}$. The deformation of a solid can be decomposed into changes of its volume and of its shape. Volume changes are given by $J = \rho_R/\rho$, where ρ_R and ρ are the mass densities in the reference state and in the actual configuration, whereas changes of the shape are described by $c^{ij} = J^{-2/3}C^{ij}$ with $\det(c^{ij}) = 1$.

4. Constitutive model

The general constitutive model for GaAs starts from a free energy density $\rho\psi = \rho\psi(T, n_1, n_2, ..., c^{ij})$, which allows the calculation of the central quantities of the thermodynamics of GaAs. These are the chemical potentials, μ_a, the Cauchy stress, σ^{ij}, the pressure, $p = -\sigma^{kk}/3$, and the second Piola - Kirchhoff stress, t^{ij}. according to, see [2] for details,

$$\mu_a = \frac{\partial\rho\psi}{\partial n_a}, \quad p = -\rho\psi + \sum_{a=1}\mu_a n_a, \quad t^{ij} = -pJ(\overset{-1}{C})^{ij} + 2J^{1/3}\frac{\partial\rho\psi}{\partial c^{t\langle i}}C^{s\rangle t}(\overset{-1}{C})^{sj}.$$

The free energy density and the chemical potentials are decomposed as $\rho\psi = \rho\psi^{\text{chem}} + \rho\psi^{\text{mech}}$ and $\mu_a = \mu_a^{\text{chem}} + \mu_a^{\text{mech}}$, respectively. We define the indicated mechanical contributions so that they are zero if the body is exclusively under homogenous hydrostatic pressure. For an illustration we give the mechanical part of the chemical potentials in the solid phase that results from the Kirchhoff - St. Venant law for the stress. We refer the reader to [2] regarding the chemical contributions and the corresponding representations in the liquid phase.

$$\mu_a^{mech}(T, \varrho, c) = -\frac{M_a}{24\bar{\rho}_S(T)}(J^{2/3}c^{ij} + 3\delta^{ij})K^{ijkl}(J^{2/3}c^{kl} - \delta^{kl}),$$

This representation differs from the existing corresponding representations of the literature, see for example Landau/Lifschitz [4]. The main difference is the appearance of linear terms in the strain $(C_{ij} - \delta_{ij})/2$, which are absent in the literature.

5. Calculation of a non-standard phase diagram

We calculate the phase diagram for a GaAs solid, which contains a single spherical droplet with radius r_I. To this end we consider isothermal processes at constant

outer pressure, and then the first and second laws of thermodynamics imply

$$\frac{d\mathcal{A}}{dt} \leq 0 \quad \text{with} \quad \mathcal{A} := \Psi + p_0 V.$$

The phase diagram relies on the extrema of the available free energy $\mathcal{A} = \Psi_S + \Psi_L + \sigma 4\pi {r_I}^2 + p_0 V$. There are five side conditions: (i) conservation of total mass of Ga and As, respectively, (ii) equal numbers of lattice sites of the three sublattices, (iii) constant number of atoms during the transition of a piece of solid into a liquid droplet.

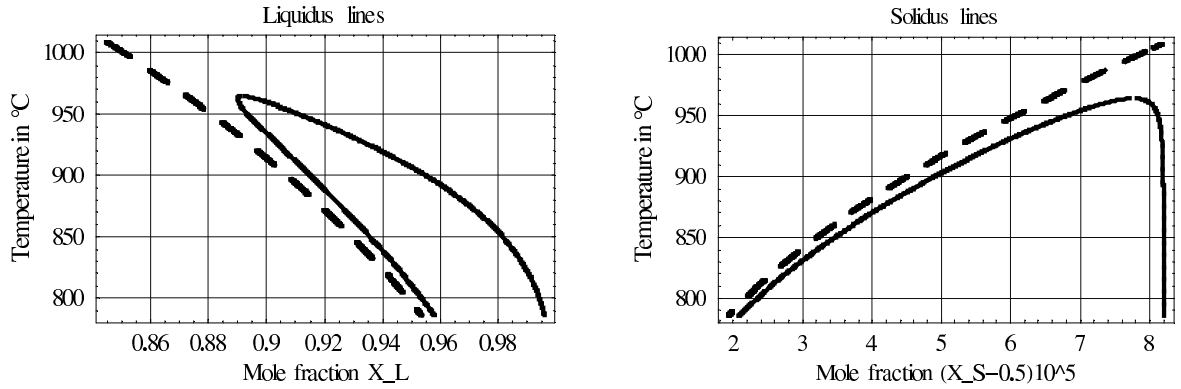

FIGURE 1

For given radius r_I there are nine unknowns: seven mole densities in the solid and two mole densities in the liquid. They are determined by the four side conditions (i) and (ii) and the necessary conditions for the minima of $\mathcal{A}$ yield five equations that read

$$\begin{aligned}
\mu_{As_\beta} - \mu_{As_\gamma} - \mu_{V_\beta} + \mu_{V_\gamma} &= 0 \\
\mu_{As_\alpha} - \mu_{As_\gamma} - \mu_{V_\alpha} + \mu_{V_\gamma} &= 0 \\
\mu_{V_\alpha} + \mu_{V_\beta} + \mu_{V_\gamma} &= 0
\end{aligned}$$

$$\begin{aligned}
\mu_{Ga_\alpha} - \mu_{Ga_L} - \mu_{V_\alpha} - \frac{M_{Ga}}{\rho_S}\sigma^{\langle ik\rangle}\nu_I^i\nu_I^k &= 0 \\
\mu_{As_\gamma} - \mu_{As_L} - \mu_{V_\gamma} - \frac{M_{As}}{\rho_S}\sigma^{\langle ik\rangle}\nu_I^i\nu_I^k &= 0
\end{aligned}$$

The deviatoric stress $\sigma^{\langle ik\rangle}$ follows from the solution of the mechanical problem of a misfitting liquid droplet in a solid environment and contains the radius of the droplet as a parameter, which, however, can be fixed by the side condition (iii). For the details see [1] and [2].

There result standard and non-standard phase diagrams. The figure on the left hand side shows the liquidus lines. The solid line represents the standard liquidus line corresponding to the minima of $\mathcal{A}$ for the standard system, whereas

the two dashed lines regard the non-standard system. The left part gives the stabil equilibria and the right part corresponds to the maxima of $\mathcal{A}$ and gives the critical radii. The figure on the right hand side shows the solidus lines. The standard system is indicated again by the solid line, and the two dashed lines represent the arsenic concentration of the solid for the stabil and unstabil equilibria, respectively. Further details are found in [3].

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Random Homogenization for Liquid-Solid Phase Transitions with Equiaxed Dendritic Microstructure

Christof Eck

Many solidification processes, for example in the casting of metals, exhibit a dendritic microstructure of the phase interface, as schematically depicted in Fig. 1. We consider the following phase field model for binary alloys:

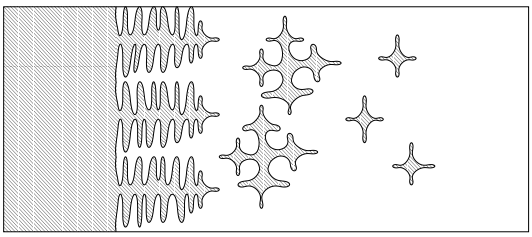

Figure 1. Columnar (left) and equiaxed (right) dendritic structures

$$
\begin{aligned}
\partial_t T + L\partial_t \Phi - \nabla \cdot (K(\Phi)\nabla T) &= 0 \\
\partial_t c - \nabla \cdot (D_1(\Phi)\nabla c) - \nabla \cdot (D_2(c,\Phi)\nabla \Phi) &= 0 \qquad (1) \\
\alpha\xi^2 \partial_t \Phi - \xi^2 \Delta \Phi + p'(\Phi) + q(\nabla\Phi, T, c, \Phi) &= 0
\end{aligned}
$$

The quantities there are temperature T, concentration c, phase field Φ, with $\Phi = 1$ in liquid and $\Phi = -1$ in solid, diffusivity constants K, D_1, D_2, half of the latent heat L, kinetic coefficient α, constitutive parameter ξ, a double well potential p and a function q related to the phase difference of a free energy or entropy.

Using techniques from homogenization theory, we derive a two-scale model that is suitable for a very small scale of equiaxed dendritic structures. The structures are generated via initial conditions that have oscillations of a given scale ε,

$$u(0,x) = u_0(x, x/\varepsilon) \text{ with } u_0 : \Omega \times Y \to \mathbb{R} \text{ for } u = T, c, \Phi,$$

with spacial domain Ω and periodicity cell Y of size 1. The data are scaled according to $D_j = \varepsilon^2 D_{j,0}$, $\xi = \varepsilon\xi_0$, $\alpha = \varepsilon^{-2}\alpha_0$ and $q(\nabla\Phi, \cdots) = q_0(\varepsilon\nabla\Phi, \cdots)$. For locally periodic structures the two-scale model consists of a global heat equation

$$\partial_t T + L\partial_t \overline{\Phi} - \nabla \cdot \big(K^*(\Phi)\nabla T\big) = 0 \tag{2}$$

for $T = T(t,x)$ with cell average $\overline{\Phi}(t,x) = \int_Y \Phi(t,x,y)\,dy$ and effective heat conductivity $K^*(\Phi)$, and of local microscopic problems

$$\begin{aligned} \partial_t c - \nabla_y \cdot \big(D_{0,1}(\Phi)\nabla_y c\big) - \nabla_y \cdot \big(D_{0,2}(c,\Phi)\nabla_y \Phi\big) &= 0 \\ \alpha_0\xi_0^2\partial_t\Phi - \xi_0^2\Delta_y\Phi + p'(\Phi) + q_0(\nabla_y\Phi, T, c, \Phi) &= 0 \end{aligned} \tag{3}$$

for $(c,\Phi) = (c,\Phi)(t,x,y)$. The microscopic problems describe the evolution of single equiaxed crystals, they are solved for every point $x \in \Omega$. The two-scale model is rigorously justified by an estimate that compares the solution $u_\varepsilon = u_\varepsilon(t,x)$, $u \in \{T, c, \Phi\}$, of the original problem of scale ε with *macroscopic reconstructions* $u^\varepsilon(t,x) = u(t,x,x/\varepsilon)$ of the solutions $u = u(t,x,y)$ of the two-scale model:

$$\sum_{u=T,c,\Phi} \|u_\varepsilon - u^\varepsilon\|_{L_\infty(I_t;L_2(\Omega))} \le C\varepsilon^{1/2}$$

In a numerical discretization of the two-scale model the mesh size is decoupled from the scale of the microstructure. The two-scale model is superior, if the mesh size for the macroscopic problem is bigger than the scale of the microstructure.

The case of a non-periodic, random microstructure is modeled by a probabilistic description of the initial conditions. Following the approach described in [4], the initial conditions are given via realizations of random fields with respect to an ergodic multi-dimensional system $\mathfrak{T}$ on a probability space $\mathfrak{P}$;

$$u(0,x) = u_0(x, \mathfrak{T}(x/\varepsilon)\omega) \text{ with } u : \Omega \times \mathfrak{P} \to \mathbb{R} \text{ for } u \in \{T, c, \Phi\}$$

with fixed $\omega \in \mathfrak{P}$. The corresponding homogenized two-scale model consists of the macroscopic heat equation (2) with the corresponding stochastic versions of the effective heat conductivity $K^*(\Phi)$ and the expectation value $\overline{\Phi}$ instead of the cell average; and of microscopic problems whose solutions are random fields $u = u(t,x,\omega)$, $\omega \in \mathfrak{P}$. The latter can be formulated as partial differential equations on $\mathbb{R}^N$ for the realizations $u^\omega(t,x,y) = u(t,x,\mathfrak{T}(y)\omega)$, $u = c, \Phi$, of these random fields. These equations are the same (3) as for the periodic case, but they are solved on the full space $\mathbb{R}^N$. It is possible to derive an estimate for the difference of the solutions $u_{\omega,\varepsilon}$ of the original problem with scale ε and choice $\omega \in \mathfrak{P}$, and the macroscopic reconstructions $u^{\omega,\varepsilon}(t,x) = u(t,x,\mathfrak{T}(x/\varepsilon)\omega)$ for the solution of the two-scale model. This difference converges to 0 for $\varepsilon \to 0$, but there is no information about the order of convergence.

In a numerical discretization of the random two-scale model one may restrict the microscopic problems to a finite domain, with suitable artificial boundary conditions. A natural choice would be periodic boundary conditions, and then the actual computation would be rather close to that for a periodic model.

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Surface diffusion driven by capillarity, stress and electromigration

Harald Garcke

(joint work with John Barrett and Robert Nürnberg)

The evolution of free surfaces driven by surface tension, mechanical stresses and/or the effect of an electric field appears in many applications. This phenomenon plays an important role in void migration in interconnects appearing in microelectronic devices and in epitaxial growth of thin films.

In the talk a sharp interface model and a phase field model are presented to model the above phenomenon. The sharp interface model is a fourth order geometric evolution equation for the interface coupled to an elliptic system which has to hold in the bulk. This system models mechanical equilibrium and determines the electric potential. If we denote by $\mathcal{E}(u)$ the linear elastic strain, by $W_1(\mathcal{E})$ the energy density and by ϕ the electric potential, the geometric evolution law is

$$V = \nabla_s \cdot D_s \nabla_s (-\sigma\kappa + W_1(\mathcal{E}(u)) + \alpha\phi)$$

where V is the normal velocity, ∇_s is the surface gradient, $\nabla_s \cdot$ is the surface divergence, D_s is a diffusion constant and σ is the surface energy density. For the displacement u, the equations of linear elasticity have to hold and ϕ solves the Laplace equation, where both ϕ and u have to attain appropriate boundary conditions.

We present an asymptotic analysis relating the above geometric evolution equation to the phase field system

$$\begin{aligned} \gamma \partial_t c &= \nabla \cdot (\tfrac{8}{\pi} D_s b(c) \nabla w), \\ w &= \sigma \tfrac{2}{\pi} (-\gamma \Delta c + \tfrac{1}{\gamma}\psi(c)) + \tfrac{1}{2} d'(c) \mathcal{C}\,\mathcal{E}(u) : \mathcal{E}(u) + \alpha\phi \end{aligned}$$

where

$$d(s) := c_0 + \tfrac{1}{2}(1 - c_0)(1 + s)$$

and $b(c) = 1 - c^2$. This system is a degenerate Cahn-Hilliard equation where c in our context is an order parameter being 1 in the solid and -1 in the void. The phase field system is, as in the case of the geometric evolution equation, coupled to an elliptic system in a non-trivial way.

We prove an existence result for the full phase field model using energy and entropy estimates and a perturbation argument giving higher integrability for the gradient of the elliptic system. Existence of a solution is achieved by showing convergence of a finite element method.

Finally we present several numerical simulations of the phase field model, showing that the model recovers several experimental observed features.

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Macroscopic pulse evolution for a nonlinear oscillator chain

Johannes Giannoulis

(joint work with Alexander Mielke)

We consider the nonlinear oscillator chain

$$\ddot{x}_j = V'(x_{j+1}-x_j) - V'(x_j-x_{j-1}) - W'(x_j), \quad j \in \mathbb{Z}, \tag{1}$$

where the potentials $V, W \in \mathrm{C}^5(\mathbb{R})$ are of the form

$$V(d) := \frac{\alpha_1}{2}d^2+\frac{\alpha_2}{3}d^3+\frac{\alpha_3}{4}d^4+\mathcal{O}(d^5), \quad W(x) := \frac{\beta_1}{2}x^2+\frac{\beta_2}{3}x^3+\frac{\beta_3}{4}x^4+\mathcal{O}(x^5). \tag{2}$$

These are the equations of motion for the deviations $x_j(t) \in \mathbb{R}$ from the rest positions $j \in \mathbb{Z}$ of (a chain of) atoms with equal mass 1, at time $t \geq 0$. V is the potential for the nearest-neighbor interaction, and W is an external potential, which might arise through embedding of the atomic chain in a background field.

The linearized system

$$\ddot{x}_j = \alpha_1(x_{j+1}-2x_j+x_{j-1}) - \beta_1 x_j, \quad j \in \mathbb{Z},$$

has the basic solutions $x_j(t) = \mathrm{e}^{\mathrm{i}(\widetilde{\omega}t+\vartheta j)}$, where the wave number $\vartheta \in (-\pi, \pi]$ and the frequency $\widetilde{\omega}$ have to satisfy the dispersion relation $\widetilde{\omega}^2 = 2\alpha_1(1-\cos\vartheta)+\beta_1 =: \omega^2(\vartheta)$. We assume $\min\{\beta_1, 4\alpha_1+\beta_1\} > 0$ in order to obtain stability: $\omega^2(\vartheta) > 0$ for all $\vartheta \in (-\pi, \pi]$. We consider a fixed value $\vartheta \in (-\pi, \pi]$, and write shortly ω, ω', ω'' to denote $\omega(\vartheta)$, $\omega'(\vartheta)$, $\omega''(\vartheta)$, respectively. The associated basic mode $\mathbf{E}(t, j) := \mathrm{e}^{\mathrm{i}(\omega t+\vartheta j)}$ is considered to be the microscopic pattern.

Our aim is to understand the macroscopic evolution of solutions, which are modulations of the microscopic pattern, given by a modulation function $A : [0,\tau_0]\times\mathbb{R} \to \mathbb{C}$:

$$(3)\quad x_j(t) = (X_\varepsilon^A)_j(t) + \mathcal{O}(\varepsilon^2) \quad \text{with} \quad (X_\varepsilon^A)_j(t) := \varepsilon A(\varepsilon^2 t, \varepsilon(j-ct))\mathbf{E}(t,j) + \text{c.c.}$$

(c.c. denotes the complex conjugate), where $\varepsilon \le \varepsilon_0$ for some $\varepsilon_0 > 0$, and where $\tau = \varepsilon^2 t$ and $\xi = \varepsilon(j-ct)$ play the role of a macroscopic time and space variable, respectively. To this end, we derive formally the associated modulation equation for A, and then justify it mathematically as a valid macroscopic limit.

Inserting (3) into the nonlinear problem (1) will generate higher harmonic terms (with factors $\mathbf{E}^n$) having scaling parameters ε^k, $k \in \mathbb{N}$. Hence, we insert in (1) the multiple scale ansatz

$$(X_\varepsilon^{(A)})_j(t) := (X_\varepsilon^A)_j(t) + \sum_{k=2,3} \varepsilon^k \sum_{n=-k}^{k} A_{k,n}(\tau,\xi)\mathbf{E}(t,j)^n$$

with $A_{k,-n} = \bar{A}_{k,n}$, and expand the left hand side and right hand side of the equation in terms of $\varepsilon^k\mathbf{E}^n$. Then we equate the coefficients of both sides for each of these terms separately. Thus, we obtain an hierarchy of equations for $k = 1,2,3,\ n = 0,\dots,k$ (cf. [1, Sec. 2]). Solving these equations consecutively, we obtain $c = -\omega'$, and can determine the functions $A_{k,n}$ as functions of A, which in turn has to be necesarilly a solution of the nonlinear Schrödinger equation (NLSE)

$$(4)\quad \mathrm{i}\partial_\tau A = \frac{1}{2}\omega''\partial_\xi^2 A + \rho|A|^2 A, \quad \rho := \frac{1}{\omega}\left(\frac{(\alpha_2 s_1 c_1)^2 - \beta_2^2}{4\omega^2 - \omega^2(2\vartheta)} + \frac{2\beta_2^2}{\beta_1} - \frac{3\left(\alpha_3 c_1^2 + \beta_3\right)}{2}\right)$$

($s_1 := 2\mathrm{i}\sin\vartheta$, $c_1 := 2(1-\cos\vartheta)$). Thus, we have shown that if the microscopic model (1) has for all $\varepsilon \le \varepsilon_0$ and $\varepsilon^2 t \le \tau_0$ solutions of the form (3), where $A : [0,\tau_0]\times\mathbb{R} \to \mathbb{C}$ is a smooth function, then A has to satisfy the NLSE (4). We call this result a formal derivation, since the existence of solutions maintaining the form (3) for $t \le \tau_0/\varepsilon^2$ is not at all clear.

The mathematical justification of the NLSE (4) consists in showing, that for A satisfying (4) for $\tau \in [0,\tau_0]$, $\tau_0 > 0$, solutions $t \mapsto (x_j(t))_{j\in\mathbb{Z}}$ of (1), which start at $t = 0$ in the form (3), stay in this form over intervals $[0,\tau_0/\varepsilon^2]$, which have a positive macroscopic length.

More precisely, we have shown the following theorem ([1, 2]):

Theorem. *Assume that the potentials V, $W \in \mathrm{C}^5(\mathbb{R})$ in (1) have the form (2) with $\min\{\beta_1, (16/3)\alpha_1+\beta_1\} > 0$. Let $A : [0,\tau_0]\times\mathbb{R} \to \mathbb{C}$, $\tau_0 > 0$, be a solution of the NLSE (4) with $A(0,\cdot) \in \mathrm{H}^5(\mathbb{R})$, and let X_ε^A be the formal approximation given in (3) with $c = -\omega'$. Then, for each $d > 0$ there exist $\varepsilon_0, C > 0$ such that for all $\varepsilon \in (0,\varepsilon_0)$ the following statement holds: Any solution x of (1) satisfying*

$$\|(x(0),\dot{x}(0)) - (X_\varepsilon^A(0),\dot{X}_\varepsilon^A(0))\|_{\ell^2\times\ell^2} \le d\varepsilon^{3/2},$$

fulfills the estimate

$$\|(x(t),\dot{x}(t))-(X_\varepsilon^A(t),\dot{X}_\varepsilon^A(t))\|_{\ell^2\times\ell^2}\le C\varepsilon^{3/2}\quad \textit{for}\quad t\in[0,\tau_0/\varepsilon^2].$$

We give a short sketch of the proof of the theorem. The details can be found in [1, 2]. In the first paper [1] we justified the NLSE (4) in the case of absence of quadratic terms in the nonlinearity. We followed the ideas used also in [3].

We write (1) as a first order system $\dot{\widetilde{x}} = L\widetilde{x} + N(\widetilde{x})$ in the Banach space $Y = \ell^2\times\ell^2$ with $\widetilde{x} := (x, \dot{x})$. Y is equipped with the energy norm $\|\cdot\|$, equivalent to $\|\cdot\|_{\ell^2\times\ell^2}$. We want to prove that the error $R := \varepsilon^{-3/2}(\widetilde{x}-\widetilde{X}_\varepsilon^A)$ between an original solution $\widetilde{x}$ and the approximation $\widetilde{X}_\varepsilon^A$ remains bounded for $t\in[0,\tau_0/\varepsilon^2]$. By definition, the error fulfills an evolution equation, which by the variation of constants formula leads to the estimate

(5)

$$\|R(t)\|\le\|R(0)\|+\varepsilon^{-3/2}\int_0^t\|N(\widetilde{X}_\varepsilon^{(A)}(s)+\varepsilon^{3/2}R(s))-N(\widetilde{X}_\varepsilon^{(A)}(s))+\mathrm{res}(\widetilde{X}_\varepsilon^{(A)}(s))\|\mathrm{d}s$$

with the residuum $\mathrm{res}(\widetilde{X}_\varepsilon^{(A)}) := \dot{\widetilde{X}}_\varepsilon^{(A)} - L\widetilde{X}_\varepsilon^{(A)} - N(\widetilde{X}_\varepsilon^{(A)})$. From the formal derivation of (4) we obtain $\mathrm{res}(\widetilde{X}_\varepsilon^{(A)}) = \mathcal{O}(\varepsilon^4)$ for $\varepsilon\to 0$ pointwise in $j\in\mathbb{Z}$. This yields $\|\mathrm{res}(\widetilde{X}_\varepsilon^{(A)})\| = \mathcal{O}(\varepsilon^{7/2})$ (cf. [1, Prop. 3.3]). On the other hand, using the cubic structure of N, we show by use of the mean value theorem the estimate

$$\|N(\widetilde{X}_\varepsilon^{(A)}(t)+\varepsilon^{3/2}R(t))-N(\widetilde{X}_\varepsilon^{(A)}(t))\|\le C_N\varepsilon^{7/2}\|R(t)\|\quad\text{as long as}\quad\|\widetilde{R}(t)\|\le D.$$

Inserting these estimates in (5), we eventually obtain the statement of the theorem by a Gronwall type argument.

In the case of presence of quadratic terms of the nonlinearity, which we treated in [2], we obviously can not apply directly the method we have just described, since it relies exactly on the absence of quadratic terms. We circumvent this difficulty by applying a method also used in [4]. It consists in applying on the original system $\dot{\widetilde{x}} = L\widetilde{x} + Q(\widetilde{x},\widetilde{x}) + M(\widetilde{x})$ (with quadratic terms Q and cubic and higher order terms M) the normal form transform $F : Y\to Y$ with $\widetilde{y} = F(\widetilde{x}) := \widetilde{x} + B(\widetilde{x},\widetilde{x})$, where $B : Y\times Y\to Y$ is a bilinear form, which has to be determined. We obtain the transformed system

$$\dot{\widetilde{y}} = L\widetilde{y}+\bar{Q}(\widetilde{x},\widetilde{x})+\bar{M}(\widetilde{x}),\quad \bar{Q}(\widetilde{x},\widetilde{x}) := -LB(\widetilde{x},\widetilde{x})+B(L\widetilde{x},\widetilde{x})+B(\widetilde{x},L\widetilde{x})+Q(\widetilde{x},\widetilde{x}),$$

where $\bar{Q}$ consists again of all quadratic terms. Next, we determine B such that $\bar{Q}\equiv 0$. This can be done uniformly for all $\vartheta\in[-\pi,\pi)$, if we restrict ourselves to the case $\min\{\beta_1,(16/3)\alpha_1+\beta_1\} > 0$. Exploiting the boundedness of B, we thus obtain the system $\dot{\widetilde{y}} = L\widetilde{y} + N(\widetilde{y})$ with $N(\widetilde{y}) := \bar{M}(F^{-1}(\widetilde{y}))$, which has a nonlinearity with cubic leading terms. Applying on this transformed system the method used in [1], we obtain an estimate for the transformed error. Transforming back, this gives us the estimate for the error R of the original system. Of course, the derivation of the estimate for the transformed error, is more complicated then in the case of absent quadratic terms in the original system, since the non-local operator B is involved in the nonlinearity N. □

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Entropy driven phase transition in a system of hard rods

Dmitry Ioffe
(joint work with Yvan Velenik, Milos Zahradnik)

We study a system of rods on $\mathbb{Z}^2$, with hard-core exclusion. Each rod has a length between 2 and N. We show that, when N is sufficiently large, and for suitable fugacity, there are several distinct Gibbs states, with orientational long-range order. This is in sharp contrast with the case $N = 2$ (the monomer-dimer model), for which Heilmann and Lieb proved absence of phase transition at any fugacity. This is the first example of a pure hard-core system with phases displaying orientational order, but not translational order; this is a fundamental characteristic feature of liquid crystals.

Our model is defined as follows. We call rod a family of k, $k \in \mathbb{N}$, distinct, aligned, nearest-neighbor sites of $\mathbb{Z}^2$ a k-rod is a rod of length k, and we refer to 1-rod as vacancies. Let $V \subset \mathbb{Z}^2$; a configuration ω of our model inside V is a partition of V into a family of disjoint rods. We write $N_k(\omega)$ the number of k-rods in ω. The probability of the configuration ω is given by

$$\mu_{q,N,V}(\omega) \propto \mathbf{1}_{\{N_k(\omega)=0,\,\forall k>N\}}(2q)^{N_1(\omega)}\, q^{\sum_{k=2}^{\infty} N_k(\omega)}\,,$$

where $q > 0$ and $N \in \mathbb{N}$. Informally, only rods of length at most N are allowed; the activity of each rod of length at least 2 is q, and is independent of the rod's length; there is an additional activity $2q$ for vacancies. Note that the activity of vacancies can be removed at the cost of introducing an additional factor $(2q)^{-k}$ for each k-rods ($k \geq 2$).

Our main task is the proof of the following theorem, which states that for large enough N, there is a phase transition from a unique (necessarily isotropic) Gibbs state at large values of q to several Gibbs states with long-range orientational order at small values of q, but *no* translational order. This is thus the first model, where such a behavior can be proved. We claim that:

1) For any $N \geq 2$, there exists $q_0 = q_0(N) > 0$ such that, for all $q \geq q_0$ there is a unique, isotropic Gibbs state.
2) There exist N_0, and q_1 such that for all $N \geq N_0$ and all $q \leq q_1$, there are 2 different extremal Gibbs states with long-range orientational order. More precisely, there exists a Gibbs state $\mu_{q,N}$ such that

$$\mu_{q,N}(\,0 \text{ belongs to a horizontal rod }) > 1/2\,.$$

The main claim 2) is proved by showing that, for N large enough, the model defined above is a small perturbation (in a suitable sense) of the "exactly solvable" case $N = \infty$. For the latter, the theorem takes the following form. Let $q_c = 1/(2 + 2\sqrt{2})$. Then:

1) Let $N = \infty$. For all $q \geq q_c$ there is a unique, isotropic Gibbs state.
2) For all $q < q_c$, there are (at least) 2 different extremal Gibbs states with long-range orientational order. More precisely, there exists a Gibbs state μ_q such that

$$\mu_q(\,0 \text{ belongs to a horizontal rod }) > 1/2\,.$$

Dynamic phase transitions in ferroic systems with pinned domain walls

Wolfgang Kleemann

Quenched randomness in ferroic systems (ferromagnets, ferroelectrics, ferroelastics) containing domain walls has interesting consequences on its response to an external conjugate field. In dependence on the strength of the driving field, h, the domain walls exhibit different states of motion below and above a critical "depinning" field, h_c, which separates the regions of thermally activated creep and friction-limited slide, respectively [1,2]. At finite frequencies, $\omega > 0$, additional states of motion are encountered: local relaxation without net wall motion at high frequencies [3] and switching between differently poled states at high field amplitudes [4]. The dynamic behavior of domain walls in random media under the influence of a periodic external field $h_0 \exp(i\omega t)$ gives rise to hysteresis cycles of different shape depending on various external parameters. According to a recent theory based on the Langevin equation of a driven interface $z(x,t)$ in a quenched random field $h_r(x,z)$ ("*Quenched Edwards-Wilkinson (QEW) equation*"[5]):

$$\gamma^{-1}(\partial z/\partial t) = \Gamma\nabla^2 z + h_0 \exp(i\omega t) + h_r(x,z) \tag{1}$$

the polarization, P, or the magnetization, M, in a disordered ferroelectric or ferromagnetic material, respectively, is expected to display a number of different features as a function of T, frequency, ω, and probing ac field amplitude, h_0. They are probably accompanied by a series of dynamical phase transitions, whose order parameters $Q = (\omega/2\pi) \oint P dt$ or $(\omega/2\pi) \oint M dt$ reflect the shape of the P or M vs. h loop. When increasing the ac amplitude h_0 the polarization or magnetization displays four regimes. First, at very low fields, $h < h_\omega$, only local "*relaxation*", but no macroscopic motion of the walls should occur at finite frequencies, $\omega > 0$.

Second, within the range $h_\omega < h_0 < h_{t1}$, a thermally activated drift motion ("*creep*") is expected, while above the depinning threshold h_{t1} the "*sliding*" regime is encountered within $h_{t1} < h_0 < h_{t2}$. Finally, for $h_0 > h_{t21}$ a complete reversal of the polarization ("*switching*") occurs in the whole sample in each half of the period, $T = 2\pi/\omega$. It should be noticed that all transition fields, h_ω , h_{t1} and h_{t2}, are expected to depend strongly on both T and ω [4].

Thus a series of dynamic phase transitions emerges in the $T - \omega - h$ parameter space. This scenario has recently been observed in the strongly disordered uniaxial "*relaxor*" ferroelectric $Sr_{1-x}Ba_xNb_2O_6$ (SBN) [6], in nanoparticular ferromagnetic "*discontinuous multilayers*" $[Co_{80}Fe_{20}$ ($t_{nominal}$=1.4nm)/Al_2O_3 (3nm)$]_{10}$ (DMIM) [7], in the isotope exchanged "*quantum ferroelectric*" $SrTi^{18}O_3$ (STO18) [8] and in periodically poled ferroelectric $KTiOPO_4$ (KTP) [9]. The main features are:

(i) High frequency and/or low field and/or low temperature relaxation spectra due to *relaxation*, which are white noise-like in DMIM or highly polydispersive in SBN, STO18 and KTP.

(ii) Intermediate frequency field and/or temperature *creep* spectra, which exhibit power law dispersion

$$\chi(\omega) = \chi_\infty(1 + (i\omega\tau)^{-\beta})$$

where $\beta \approx 2/3$. This exponent was introduced semi-empirically within a theory of sideways wall motion induced susceptibility [6] as a consequence of the nonlinearity of the creep velocity, $v = v_0 exp[-\alpha(h_c/h)^\delta]$ [1]. In a very recent attempt to describe creep-induced domain wall susceptibility directly via the above QEW equation of motion (1), Fedorenko *et al.* [10] justified the exponent β by a broad distribution of mobilities, $\mu(h)$.

(iii) Low frequency and/or high field and/or high temperature *easy slide* spectra in DMIM and STO18.

(iv) Very low frequency and/or high field and/or high temperature *switching* spectra in DMIM, which obey Debye-type monodispersivity

$$\chi(\omega) = \chi_\infty(1 + i\omega\tau)^{-1}.$$

While theory has so far been applied only to the time domain [4], we have recently attempted its translation into the frequency domain by appropriate Fourier transformation [11] in order to interpret available complex linear susceptibility experiments [6,7]. We have used two different approaches.

Method (i) employs an expression for the mean domain wall velocity in the adiabatic driving regime, which interpolates between the creep and viscous sliding regime at small frequencies [4]. The mean displacement $Z(t)$ of the domain wall is related to $\partial Z/\partial t = v(H(t))$ and to the dynamic magnetization $M(t) = M_s(2Z(t)/L_z - 1)$. The simulated hysteresis curves in this adiabatic regime exhibit both the slide and the switching regime, but do not account for creep and relaxation.

Method (ii) employs the QEW equation of motion (1) of the domain wall in the non-adiabatic driving regime under random forces $h_r(x, z)$ with $< h_r >= 0$.

Numerical integration of the simulated *ac* susceptibility components in the non-adiabatic regime for frequencies $10^{-4} < f < 10^4$ Hz yields three regimes, *creep, slide* and *switching* at sub-threshold fields $h_o = 0.8\ \mathrm{h}_p$. In corroboration of the experimental data, however, all expected phase transitions are obviously thermally smeared. This is known theoretically from the creep-to-slide transition at non-zero temperature [1]. Very probably only the relaxation-to-creep transition might be unsmeared at finite temperatures as seems to be evident from sharp kinks found at h_ω in the Cole-Cole diagrams of SBN [6], DMIM [7] and KTP [9]. Unfortunately its adequate treatment is out of reach within the present model, which does not account for the local response of the domain wall to the external field.

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Annealed deviations for random walk in random scenery

Wolfgang König
(joint work with N. Gantert and Z. Shi)

Let $(Z_n)_{n\in\mathbb{N}_0}$ be a d-dimensional *random walk in random scenery*, i.e., $Z_n = \sum_{k=0}^{n-1} Y(S_k)$ with $(S_k)_{k\in\mathbb{N}_0}$ a random walk in $\mathbb{Z}^d$ and $(Y(z))_{z\in\mathbb{Z}^d}$ an i.i.d. scenery, independent of the walk. The walker's steps are assumed to have mean zero and finite variance. For the purpose of this abstract, let S be simple random walk.

The random walk in random scenery has been introduced and analyzed in dimension $d \neq 2$ by H. Kesten and F. Spitzer [3] and by E. Bolthausen [2] for $d = 2$. Under the assumption that $Y(0)$ has expectation zero and variance $\sigma^2 \in (0, \infty)$,

their results imply that

$$\frac{1}{n}Z_n \approx a_n^0 = \begin{cases} n^{-\frac{1}{4}} & \text{if } d=1, \\ (\frac{n}{\log n})^{-\frac{1}{2}} & \text{if } d=2, \\ n^{-\frac{1}{2}} & \text{if } d \geq 3. \end{cases} \tag{1}$$

More precisely, $\frac{1}{na_n^0}Z_n$ converges in distribution towards some non-degenerate random variable. In terms of the so-called *local times* of the walk,

$$\ell_n(z) = \sum_{k=0}^{n-1} \mathbb{1}_{\{S_k=z\}}, \qquad n \in \mathbb{N}, \;\; z \in \mathbb{Z}^d, \tag{2}$$

the random walk in random scenery may be identified as

$$Z_n = \sum_{z\in\mathbb{Z}^d} Y(z)\ell_n(z) = \langle Y, \ell_n \rangle. \tag{3}$$

It is the goal of the present work to identify the speed and the rate of the logarithmic decay of $\mathbb{P}(\frac{1}{n}Z_n > b_n)$ for various choices of sequences $(b_n)_n$ in $(0,\infty)$ satisfying $b_n \gg a_n^0$. Furthermore, we want to explain, at least on a heuristic level, the optimal joint strategy of the random walk and the scenery to meet the event $\{\frac{1}{n}Z_n > b_n\}$ in the cheapest way.

In order to demonstrate the main idea of the investigation, let us derive a lower bound for $\mathbb{P}(\frac{1}{n}Z_n > u)$ for $u > 0$ fixed. Our ansatz is to fix a scale function $1 \ll \alpha_n \ll n^{\frac{1}{d}}$ and to consider the event that the appropriately normalized rescaled local times and the rescaled scenery resemble fixed given shape functions $\psi^2, \varphi\colon \mathbb{R}^d \to [0,\infty)$, respectively, where we impose the conditions $\int \psi^2 = 1$ and $\langle \psi^2, \varphi \rangle \geq u$. This gives the lower bound

$$\begin{aligned} \mathbb{P}(\tfrac{1}{n}Z_n > u) &\geq \mathbb{P}\Big(\frac{\alpha_n^d}{n}\ell\big(\lfloor \cdot\, \alpha_n \rfloor\big) \approx \psi^2(\cdot), Y\big(\lfloor \cdot\, \alpha_n \rfloor\big) \approx \varphi(\cdot)\Big) \\ &\approx \exp\Big\{-\frac{n}{\alpha_n^2} I(\psi^2)\Big\} \exp\Big\{-\alpha_n^d J_H(\varphi)\Big\}, \end{aligned} \tag{4}$$

where the last line follows from well-known techniques in large-deviation theory, and the rate functions are

$$I(\psi^2) = \frac{1}{2}\|\nabla\psi\|_2^2 \qquad \text{and} \qquad J_H(\varphi) = \int \sup_{t>0}\Big(\varphi(x)t - H(t)\Big)\,\mathrm{d}x,$$

and $H(t) = \mathbb{E}(e^{tY(0)})$ is the cumulant generating function of the scenery. From (4) we already see that the choice $\alpha_n = n^{1/(d+2)}$ is the proper choice for which we can expect a non-trivial result. Indeed, A. Asselah and F. Castell [1] derived a theorem on the logarithmic asymptotics of $\mathbb{P}(\frac{1}{n}Z_n > u)$ for the case of *bounded* sceneries Y, which we do not cite here.

However, we are interested in sceneries *unbounded* from above. In general, the random walk in random scenery with unbounded sceneries has interesting relations to self-intersection properties of the walk, which makes this subject particularly

interesting. As an example, if the scenery is standard Gaussian, then the distribution of Z_n given the random walk is equal to a centred Gaussian with variance equal to $\sum_{z\in\mathbb{Z}^d} \ell_n(z)^2$, the self-intersection number.

Our main result is the following.

Theorem. Suppose that $\log \mathbb{P}(Y(0) > r) \sim -Dr^q$ as $r \to \infty$, for some $D > 0$ and $q > \frac{d}{2}$. Pick a sequence $(b_n)_{n\in\mathbb{N}}$ satisfying $1 \ll b_n \ll n^{\frac{1}{q}}$. Then

$$\lim_{n\to\infty} n^{-\frac{d}{d+2}} b_n^{-\frac{2q}{d+2}} \log \mathbb{P}\Big(\frac{1}{n} Z_n > b_n\Big) = -K_{D,q}, \tag{5}$$

where

$$K_{D,q} \equiv \inf\Big\{\frac{1}{2}\|\nabla\psi\|_2^2 + D\|\psi^2\|_p^{-q} \colon \psi \in H^1(\mathbb{R}^d), \|\psi\|_2 = 1\Big\}, \tag{6}$$

(where $\frac{1}{p} + \frac{1}{q} = 1$), and $K_{D,q}$ is positive.

The constant $K_{D,q}$ is zero in the subcritical cases where $q < \frac{d}{2}$:

Proposition (Positivity of $K_{D,q}$). Fix $d \in \mathbb{N}$ and $p, q > 1$ satisfying $\frac{1}{p} + \frac{1}{q} = 1$. Then, for any $D > 0$,

$$K_{D,q} = (d+2)\Big(\frac{D}{2}\Big)^{\frac{2}{d+2}} \Big(\frac{\chi_{d,p}}{d}\Big)^{\frac{d}{d+2}}, \tag{7}$$

where

$$\chi_{d,p} = \inf\Big\{\frac{1}{2}\|\nabla\psi\|_2^2 \colon \psi \in H^1(\mathbb{R}^d) \colon \|\psi\|_2 = 1 = \|\psi\|_{2p}\Big\}, \tag{8}$$

Moreover, the constant $\chi_{d,p}$ is positive if and only if $d \le \frac{2p}{p-1} = 2q$.

The constant $\chi_{d,p}$ is directly related to the well-known *Gagliardo-Niremberg* constant. In [6], the existence of a minimizer in (8) has been established; indeed there is a minimizer which is rotationally symmetric, positive everywhere and infinitely often differentiable. Uniqueness of the minimizer has been proven in [5] for $d \in \{2, 3, 4\}$ for all $p \in (1, \frac{d}{d-2}]$ and for $d \in \{5, 6, 7\}$ for $p \in (1, \frac{8}{d})$.

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Diffusion and domain walls

William T. Lee
(joint work with E.K.H. Salje and U. Bismayer)

A number of experimental and simulation results suggest that diffusion in twin walls is quite different from bulk diffusion. The most dramatic of these concerns sodium diffusion in WO_3 [1]. Here sodium was diffused in from the surface, and penetrates a considerable distance into the bulk following linear features which are the twin walls of the structure. There are three possible explanations why diffusion in twin walls should be faster than bulk diffusion

1. There are secondary strains within the twin wall which give it a more open structure.
2. The twin wall is elastically soft with respect to the bulk.
3. There is a large vacancy concentration within the twin wall.

Probably the most important of these is point (3). We therefore investigated the interaction between point defects such as vacancies with twin walls. We were also interested in investigating a recent experiment [2] in which the widths of twin walls in $PbTiO_3$ were measured using atomic force microscopy (AFM). The results suggested that the twin wall width was not a material constant but a function of position. They proposed the explanation that the variations in wall width was due to the dissolution of point defects within the wall. To investigate this possibility we considered a system in which an continuous order parameter $Q \in [-1, 1]$ interacts with an Ising spin $S = \pm 1$ representing a point defect. $S = +1$ signals the presence of the point defect, $S = -1$ signals its absence.

Experimentally point defects in ferroelastic crystals are known to order at very high temperatures, while the equilibration of the point defect concentration is slow, so that non-equilibrium concentrations are common. Therefore we decided to simulate the system using the microcanonical or NVT ensemble. The equation describing the energy of the system is

$$F = \sum_i \left[\frac{a}{2} \left(Q_i^2 - 1\right)^2 + \frac{\lambda}{2} \left(Q_i^2 - 1\right) \left(S_i + 1\right) \right] + \sum_{<ij>} \left[\frac{g}{2} \left(Q_i - Q_j\right)^2 + J S_i S_j \right]$$

The first term is a double well potential in the order parameter Q, the second term is the lowest order coupling between the order parameter and the point defects. The parameter λ controls the interaction between point defects and the twin wall and their effect on the wall width. The third term is a Ginzburg energy, preventing rapid spatial variations in the order parameter: in the absence of point defects this term controls the twin wall width.

In order for point defects to cause significant variations in the wall we must have an attraction between point defects and the wall (this also ensures that the point defects can affect the wall width) and furthermore the particles must cluster in the wall. This is achieved by a positive value of λ and a negative value of J.

(a) Q (b) S

FIGURE 1. Results of simulations for a point in parameter space in which defects are expected to cluster within the wall. (a) The order parameter Q dark shading corresponds to Q close to zero, i.e. twin walls, light shading corresponds to Q close to ± 1. (b) The point defect distribution. Sites of point defects are shown in black.

The clusters of point defects may be considered as nuclei of a second, defect rich phase, with an interfacial energy determined by J.

To simulate this system we used monte-carlo methods. At every stage of the monte-carlo algorithm we relaxed the order parameter Q using a conjugate gradient minimiser. Our system sizes were 40×40 sites, with 80 point defects. We carried out 500 000 Monte Carlo steps in each simulation. Figure 1 shows the resulting distribution of the spins and order parameter under conditions in which defects cluster within the wall. This shows that the clustering of point defects within the wall can have a large effect on the twin wall width.

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Rate–independent models of phase transition

ALEXANDER MIELKE

1. MECHANICAL MODELING OF RATE-INDEPENDENT PROCESSES

We consider materials which have elastic as well as inelastic behavior, the latter one being described by an internal variable z as in the theory of rate-independent, generalized standard materials. Such models for phase transitions in shape-memory alloys have been used succesfully in [2, 3, 6, 9, 10, 11].

We consider a body $\Omega \subset \mathbb{R}^d$ which undergoes a deformation $\boldsymbol{\varphi} : \Omega \mapsto \mathbb{R}^d$ such that the deformation gradient $\mathbf{F}(x) := \mathrm{D}\boldsymbol{\varphi}(x) \in \mathbb{R}^{d\times d}$. Additionally there are internal variables $z = (z^1, \ldots, z^n) \in Z \subset \mathbb{R}^n$ where Z denotes a manifold like, for instance, $\mathrm{SL}(d) \times \mathbb{R}^m \subset \mathbb{R}^{d\times d} \times \mathbb{R}^m$ in elasto-plasticity. The elastic properties are described via the elastic potential W which is a function of the

material point $x \in \Omega$ and $(\mathbf{F}, z)$: $W = \widehat{W}(x, \mathbf{F}, z)$. For fixed (x, z) we assume polyconvexity as well as coercivity. The total elastic and potential energy of a given state $(\boldsymbol{\varphi}, z) : \Omega \mapsto \mathbb{R}^d \times Z$ at time t is the Gibbs' energy:

$$\mathcal{E}(t, \boldsymbol{\varphi}, z) = \int_\Omega \widehat{W}(x, \mathrm{D}\boldsymbol{\varphi}(x), z(x))\,\mathrm{d}x - \langle \ell(t), \boldsymbol{\varphi}\rangle$$

with

$$\langle \ell(t), \boldsymbol{\varphi}\rangle = \int_\Omega \boldsymbol{f}_{\mathrm{vol}}(t, x) \cdot \boldsymbol{\varphi}(x)\,\mathrm{d}x + \int_{\Gamma_{\mathrm{Neu}}} \boldsymbol{f}_{\mathrm{tract}}(t, y) \cdot \boldsymbol{\varphi}(y)\,\mathrm{d}a(y).$$

Changes of the internal variables during a slow loading or unloading process will give rise to internal friction which dissipates energy via the rate $\dot{z}$:

$$\psi = \widehat{\psi}(x, z, \dot{z}) \geq 0 \text{ where } \dot{z}(t, x) = \tfrac{\partial}{\partial t} z(t, x).$$

The function $\widehat{\psi} : \Omega \times \mathrm{T}Z \mapsto [0, \infty]$ is called *dissipation potential*, since its derivative with respect to the rate $\dot{z}$ gives the frictional forces arising from changing z. Rate-independence is modeled by the assumption of homogeneity in $\dot{z}$ of degree 1: $\widehat{\psi}(x, z, \alpha\dot{z}) = \alpha\widehat{\psi}(x, z, \dot{z})$ for $\alpha \geq 0$. Thus, $\widehat{\psi}(x, \cdot, \cdot)$ defines a distance on Z via

$$\widehat{D}(x; z_0, z_1) = \inf\{\, \textstyle\int_0^1 \widehat{\psi}(x, z(s), \dot{z}(s))\,\mathrm{d}s \mid z \in \mathrm{C}^1([0,1], Z), z(0) = z_0, z(1) = z_1 \,\}.$$

This defines also a metric on the set of internal states $\mathcal{Z}$ by setting, for $z_0, z_1 \in \mathcal{Z}$, $\mathcal{D}(z_0, z_1) = \int_\Omega \widehat{D}(x; z_0(x), z_1(x))\,\mathrm{d}x$. The distance $\mathcal{D}$ is called the *dissipation distance* between the internal states z_0 and z_1 in $\mathcal{Z}$. By definition the functions $\widehat{D}(x, \cdot, \cdot)$ and hence the function $\mathcal{D}$ satisfy the triangle inequality $\mathcal{D}(z_0, z_2) \leq \mathcal{D}(z_0, z_1) + \mathcal{D}(z_1, z_2)$ for $z_0, z_1, z_2 \in \mathcal{Z}$. We note that we never assume that $\widehat{\psi}(x, z, \cdot)$ is symmetric, i.e., in general $\mathcal{D}(z_0, z_1) \neq \mathcal{D}(z_1, z_0)$. Such an unsymmetry is needed to describe damage or hardening in plasticity.

The dissipation along a curve $z : [0, T] \mapsto \mathcal{Z}$ can be expressed without any rate via $\mathrm{Diss}(z, [t_0, t_1]) = \sup \sum_{i=1}^M \mathcal{D}(z(\tau_{i-1}), z(\tau_i))$ where the supremum is taken over all discretizations.

Definition 1. A process $(\boldsymbol{\varphi}, z) : [0, T] \mapsto \mathcal{F} \times \mathcal{Z}$ is called an *energetical solution* of the rate-independent problem associated to $(\mathcal{F} \times \mathcal{Z}, \mathcal{E}, \mathcal{D})$, if the *stability condition* (S) and the *energy balance* (E) hold for all $t \in [0, T]$:

(S) $\mathcal{E}(t, \boldsymbol{\varphi}(t), z(t)) \leq \mathcal{E}(t, \widehat{\boldsymbol{\varphi}}, \widehat{z}) + \mathcal{D}(z(t), \widehat{z})$ for all $(\widehat{\varphi}, \widehat{z}) \in \mathcal{F} \times \mathcal{Z}$.

(E) $\mathcal{E}(t, \boldsymbol{\varphi}(t), z(t)) + \mathrm{Diss}(z; [0, t]) = \mathcal{E}(0, \boldsymbol{\varphi}(0), z(0)) + \int_0^t \frac{\partial}{\partial \tau}\mathcal{E}(\tau, \boldsymbol{\varphi}(\tau), z(\tau))\,\mathrm{d}\tau.$

The stability condition (S) has a clear mechanical interpretation. Letting $\widehat{z} = z(t)$ we have $\mathcal{D}(z(t), \widehat{z}) = 0$ and the condition implies that $\boldsymbol{\varphi}(t)$ is a global minimizer of $\mathcal{E}(t, \cdot, z(t))$ on $\mathcal{F}$, which gives elastic equilibrium. Moreover, any change of $z(t)$ into $\widehat{z}$ must dissipate at least as much energy as the associated gain in the elastic energy. Thus, (S) is equivalent to a principle of maximal dissipation. The internal variable will move (and dissipate energy) as soon as the energy release in the elastic energy is large enough to compensate for the dissipation. The energy inequality (E) has an obvious interpretation, since $\frac{\partial}{\partial t}\mathcal{E}$ is the power of the changing external forces.

2. Abstract existence theory

Defining the reduced potential $\mathcal{I}(t,z) = \inf\{\, \mathcal{E}(t,\boldsymbol{\varphi},z) \mid \boldsymbol{\varphi} \in \mathcal{F} \,\}$ the mathematic can be formulated most consistently. In [8] it is shown that this form is equivalent to (S) and (E) under reasonable assumptions on Ψ and $\mathcal{E}$. In [7, 8] an existence theory for (S) and (E) was developed under the assumption that $\mathcal{Z}$ is a weakly closed, convex subset of a Banach space X and that $\mathcal{D}$ is given in the form $\mathcal{D}(z_0,z_1) = \Psi(z_1 - z_0)$.

Here we present the more general approach of [1, 4] which is independent of any linear structure in $\mathcal{Z}$. The phase space $\mathcal{Z}$ is considered to be a topological space like a weakly closed subset of a Banach space. The dissipation distance $\mathcal{D} : \mathcal{Z} \times \mathcal{Z} \to [0,\infty]$ is continuous, satisfies the triangle inequality and the following compatibility with the topology on $\mathcal{Z}$: if $\min\{\mathcal{D}(z,z_k), \mathcal{D}(z_k,z)\} \to 0$ for $k \to \infty$, then $z_k \overset{\mathcal{Z}}{\to} z$. The functional $\mathcal{I} : [0,T] \times \mathcal{Z} \to \mathbb{R} \cup \{\infty\}$ has compact sublevels and is differentiable in t such that there exist constants $C_I, I_0 > 0$ with $|\frac{\partial}{\partial t}\mathcal{I}(t,z)| \le C_I(I_0 + \mathcal{I}(t,z))$ whenever $\mathcal{I}(t,z) < \infty$.

One of the standard methods to obtain solutions of nonlinear evolution equations is that of approximation by time discretizations. To this end we let $t_k^N = kT/N$ for $k = 0, 1, \dots, N$ and seek z_k which approximates z at t_k^N. The energetical formulation suggests the following incremental problem.

(IP) *For $z_0 \in \mathcal{S}(0) \subset \mathcal{Z}$ find $z_1, \dots, z_N \in \mathcal{Z}$ such that*
$z_k \in \operatorname{Argmin}\{\, \mathcal{I}(t_k,z) + \mathcal{D}(z_{k-1},z) \mid z \in X \,\}$ *for $k = 1, \dots, N$.*

Here "Argmin" denotes the set of all minimizers and $\mathcal{S}(t) = \{z \in \mathcal{Z} \mid \mathcal{I}(t,z) \le \mathcal{I}(t,\widehat{z}) + \mathcal{D}(z,\widehat{z})$ for all $\widehat{z} \in \mathcal{Z}\}$ is the set of stable states, such that (S) can be written as $z(t) \in \mathcal{S}(t)$. It is easy to dereive the a priori estimate $\mathcal{I}(t_k,z_k) + \sum_{j=1}^k \mathcal{D}(z_{j-1},z_j) \le C(z_0,T)$ (independent of k and N). This supplies compactness of the interpolants for each $t \in [0,T]$ as well a BV-type estimate on $[0,T]$ via the dissipation.

Theorem 2. *For each $z_0 \in \mathcal{S}(0)$ (S) and (E) have at least one solution.*

3. Applications in Phase Transformations in Shape-Memory Alloys

In each microscopic point y, an elastic material is free to choose one of p crystallographic phases and that the elastic energy density W is then given by $W_j(\mathrm{D}\phi)$. On the mesoscopic level, the internal variables are phase portions $z^{(j)} \in [0,1]$ for the j-th phase and we set $Z = \{\, z \in [0,1]^p \subset \mathbb{R}^p \mid \sum_1^p z^{(j)} = 1 \,\}$ and $\mathcal{Z} = \mathrm{L}^1(\Omega, Z)$. The material properties are described by a mixture function $W : \mathbb{R}^{d\times d} \times Z \to [0,\infty]$, see [9, 2] and the dissipation has the form $D(z_0,z_1) = \widehat{\psi}(z_1 - z_0)$. So far we are unable to prove existence results for this model in its full generality. However, the case with only two phases ($p = 2$) was treated successfully in [9] under the additional assumption that the elastic behavior is linear and both phases have the same elastic tensor.

In [5] a microscopic model is treated where no phase mixtures are allowed, i.e., $z \in Z_p := \{e_1, e_2, \dots, e_p\} \subset \mathbb{R}^p$, where e_j is the j-th unit vector. The functions

$z \in \mathcal{Z}$ are like characteristic functions which indicate exactly one phase at each material point. The dissipation is as above, but now the elastic energy contains an additional term measuring the surface area of the interfaces between the different regions: $\mathcal{E}(t, \boldsymbol{\varphi}, z) = \int_\Omega W(\mathrm{D}\boldsymbol{\varphi}, z)\,\mathrm{d}x + \sigma \int_\Omega |\mathrm{D}z| - \langle \ell_{\mathrm{ext}}(t), \boldsymbol{\varphi} \rangle$, where σ is a positive constant. Here $\mathcal{Z} = \{\, z : \Omega \to Z_p \mid \int_\Omega |\mathrm{D}z| < \infty \,\}$ equipped with the L^1-topology.

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Socio-thermodynamics – Integration and segregation in a population

Ingo Müller

An analogy is constructed between thermodynamics and sociology. The sociological system is one of hawks and doves who compete for the same resource. In the analogy the price of the resource corresponds to the temperature of a liquid or solid and the two species correspond to the constituents of a liquid solution or an alloy. Different phases of a solution are analogous to different strategies of competition in the population. It turns out that in good times, when the price is low the species mix homogeneously while in bad times when the price is high, there is segregation into hawk-rich and dove-rich colonies.

A life-long preoccupation with thermodynamics has given me the fixed idea that thermodynamic concepts and thermodynamic arguments may be used in fields outside physics. As a result I believe that the average behaviour of large systems of

many individual elements follows a predictable course which represents a compromise between the attraction of the individuals on the one hand and their tendency to spread out by random walk on the other hand.

Once this idea is conceived analogies appear between

- a system of atoms that seeks to minimize its potential energy and to maximize its entropy.
- a population of birds in search for a needed resource and competing for it, and
- the evolution of species hunting the same prey.

Such analogies call for the introduction of thermodynamic thinking into sociology and socio-biology.

The fact is that thermodynamics is fully understood for more than a century and a half. And in thermodynamics the knowledge about the conflicting interests between individual atoms sticking to each other and the system seeking equal distribution of the atoms over all available space have long jelled into the concepts of low energy, high entropy, and low free energy.

Thus it is well-known under which pressures and temperatures two liquids, say water and propylenoxide, form a homogeneous solution and under what circumstances they do *not* mix so that droplets of propylenoxide appear in a bulk of water like fat droplets in a watery soup.

It is less well-known under what conditions a population of two species live together harmoniously and homogeneously mixed, i.e. in a fully integrated manner, and what the conditions are for the species to segregate into colonies with a large majority of one or the other.

This is the question which I plan to address in the present work and for that purpose I consider a bird population with two characters: hawks and doves both competing for the same resource.

For the record I will say that these hawks and doves are not real hawks and doves. In particular, the hawks do not eat the doves. The species are more like the hawks and doves in the Pentagon of the United States. Infact my hawks and doves are an often used paradigm for a mixed population in game theory. I believe that the rules of the game were invented by Maynard-Smith & Price [1]. They are used in socio-biology by Dawkins [2] and in the same context the game is described by Straffin [3].

Remark: Preliminary and much less detailed versions of socio-thermodynamics were published in my articles [4] and [5] dedicated to Professors K.H. Hoffmann and K. Hutter respectively in celebration of their 60^{th} birthdays.

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Droplet growth for isotropic and anisotropic model with Kawasaki dynamics

Francesca Romana Nardi

(joint work with E. Olivieri and E. Scoppola, A. Bovier and F. den Hollander)

We analyze metastability and nucleation in the context of a "local version" of the Kawasaki dynamics for the two-dimensional Ising lattice gas at very low temperature.

Let $\Lambda \subset \mathbb{Z}^2$ be a sufficiently large finite box and let $\partial^- \Lambda = \{x \in \Lambda \colon \exists\ y \notin \Lambda \colon |y-x| = 1\}$, be the interior boundary of Λ and let $\Lambda_0 = \Lambda \setminus \partial^- \Lambda$ be the interior of Λ. With each $x \in \Lambda$ we associate an occupation variable $\eta(x)$, assuming values 0 or 1. A lattice configuration is denoted by $\eta \in \mathcal{X} = \{0,1\}^\Lambda$. Each configuration $\eta \in \mathcal{X}$ has an energy given by the following Hamiltonian:

$$H(\eta) = -U_1 \sum_{(x,y)\in\Lambda^*_{0,h}} \eta(x)\eta(y) - U_2 \sum_{(x,y)\in\Lambda^*_{0,v}} \eta(x)\eta(y) + \Delta \sum_{x\in\Lambda} \eta(x)$$

where $\Lambda^*_{0,h}$ (resp. $\Lambda^*_{0,v}$) is the set of the horizontal (vertical) unoriented bonds joining n.n. points in Λ_0. Thus the interaction is acting only inside Λ_0; the binding energy associated to a horizontal (vertical) bond is $-U_1 < 0$ ($-U_2 < 0$). We say that $U_1 = U_2$ corresponds to the isotropic case. We will refer to $U_1 \neq U_2$ as anisotropic case and we suppose without loss of generality that $U_1 > U_2$.

Kawasaki dynamics is a discrete time Markov chain on the state space $\mathcal{X}$, defined by Metropolis algorithm in such a way that: on the finite box Λ_0, particles live and evolve in a conservative way, and at the boundary $\partial^-\Lambda$, are created with rate $\rho = e^{-\Delta\beta}$ resp. annihilated with rate 1. Where β is the inverse temperature and $\Delta > 0$ is an activity parameter. Thus, the boundary of Λ plays the role of an infinite gas reservoir with density ρ. We take $\Delta \in (U_1, U_1 + U_2)$ where the totally empty (full) configuration can be naturally associated to metastability (stability). In this way the number of particles is not globally conserved and the equilibrium will be described by means of a grancanonical Gibbs measure with a chemical potential which is related to the rate of creation of particles at the boundary. The detailed balance condition is satisfied with respect to the Gibbs grancanonical measure corresponding to the Hamiltonian. We consider the asymptotic regime corresponding to fixed volume and chemical potential in the limit of large inverse temperature β. The above setup gives rise to a reversible Freidlin Wentzell Markov chain.

For the *isotropic case* we discuss the results in [1], where we study the metastable behavior of the model in two and three dimensions. We are interested in how the system nucleates, i.e., how it reaches a full box when it starts from an empty box. Our approach combines geometric and potential theoretic arguments. Our goal is to improve on earlier work by combining a detailed analysis of the energy landscape for the dynamics with the potential theoretic approach to metastability that was developed in Bovier, Eckhoff, Gayrard, and Klein [2].

Our main theorems sharpen those obtained by den Hollander, Olivieri, and Scoppola [3] in two dimensions and by den Hollander, Nardi, Olivieri, and Scoppola [4] in three dimensions. In particular, in two dimensions we identify the full geometry of the set of critical droplets defined in [3], compute the average nucleation time up to a multiplicative factor that tends to one in the limit of low temperature and low density, express the proportionality constant in terms of certain capacities associated with simple random walk, and compute the asymptotic behavior of this constant as the system size tends to infinity. In three dimensions, we obtain similar results but with no better control than in [4] over the geometry, and so, less control on the constant.

Kawasaki differs from Glauber in that it is *a conservative dynamics*: particles are conserved in the interior of the box. This creates a complication in controlling the growing and the shrinking of droplets, because particles have to travel between the droplet and the boundary of the box. Moreover, it turns out that in the metastable regime *particles move along the border of a droplet more rapidly than they arrive from the boundary of the box*. This leads to a shape of the critical droplet that is more complicated than the one for Ising spins under Glauber dynamics. This complexity needs to be handled in order to obtain the sharp asymptotics. For a critical comparison of Glauber and Kawasaki we refer to [6].

For the *anisotropic case* we discuss results in [7] where we identify the size and shape of the critical droplet and the time of its creation in the same limit. In particular we are able to determine the asymptotic behavior in probability, for large β, of the transition time between the empty and full configuration. Indeed, using [6], the control of the transition time can be obtained on the basis of relatively weak hypotheses: a rough knowledge of the global saddles between the metastable and the stable state together with the absence of too "deep wells".

We also have some partial information on the typical trajectories realizing the transition between metastability and stability. Indeed we discuss in detail the critical droplet representing the "gate" to the stable state. Our results are comparable but less complete with those obtained by Kotecký and Olivieri in [5] for the Ising model subject to Glauber dynamics, because we do not obtain a complete description of the tube of typical trajectories.

Let us now discuss the motivations and the specific features of our model by outlining the main results. In the Freidlin Wentzell regime it is natural to call Wulff shape the one minimizing the energy of a droplet at fixed volume. In our case this is a rectangle with horizontal and vertical sides proportional, respectively, to the corresponding coupling constants U_1 and U_2 (see [5]). The main question

that is natural to address concerns the relevance of Wulff shape in the nucleation pattern. Since, particles can move along the border of a droplet more rapidly than they can arrive from the boundary of the container, one could be tempted to conjecture that this displacement along the border of the growing droplet should be able to establish the equilibrium shape at fixed volume namely, the Wulff shape. However, a careful comparison between time scales of contraction, growth and of different types of movements on the border, shows that the above conjecture is false. The critical configurations are different and more complicated than the one for Ising spins under Glauber dynamics. We observe very different behavior of our model for weak or strong anisotropy, corresponding, roughly speaking, to U_1 smaller or larger than $2U_2$.

For weak anisotropy a rigorous result that we are able to prove is that the critical droplet is almost Wulff (with a highly degenerate and complicated microscopic structure) whereas we have strong indications that during the other stages of nucleation, namely both in the subcritical and supercritical part, the shape of the growing droplet is not Wulff. Actually large supercritical droplets tend to have almost squared shape contrary to what happens for the non conservative Glauber dynamics. In the strongly anisotropic case the critical droplet is not Wulff and Wulff shape is crossed during the supercritical growth. In any case Wulff shape is not relevant in the nucleation pattern, similarly to what came out in the Glauber case (see [5]). In any case we find that Wulff shape is not relevant for the nucleation pattern.

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Convergence to Mullins-Sekerka motion for phase kinetics equation with a conservation law

Enza Orlandi
(joint work with E.A.Carlen, M.C.Carvalho)

The nonlocal and nonlinear evolution equation I consider is typified by

$$\frac{\partial}{\partial t}m(x,t) = \nabla \cdot \big(\nabla m(x,t) - \beta(1-m(x,t)^2)(J \star \nabla m)(x,t)\big), \tag{1}$$

where $\beta > 1$ and "$\star$" denotes convolution. Moreover, J is a smooth spherically symmetric probability density with compact support. This equation first appeared in the literature in a paper [9] on the dynamics of Ising systems with long–range interaction and so–called "Kawasaki" or "exchange" dynamics. Later it was rigorously derived in [5]. In this physical context, $m(x,t) \in [-1,1]$ is the magnetization density at x at time t, viewed on the length scale of the interaction, and β is the inverse temperature. We refer to the previous quoted paper and to [8] for more physical insights. The purpose of this talk is to present a method for constructing approximate solutions to (1) suitable for studying its sharp interface limit. The sharp interface limit of (1) has been investigated by Giacomin and Lebowitz [6] using a formal analysis with matched asymptotic expansions in analogy with Pego's treatment for the Cahn-Hilliard equations, [7]. In [6], two time scales were considered: one leading to the sharp interface Stefan problem, the other, a longer time scale, leading to the Mullins-Sekerka motion. Nicolas Dirr, [4], has rigorously studied the first case for (1), by matched asymptotic expansions. In a recent paper, [3], by an alternative method, it has been shown how to construct an approximate solutions to a class of evolutions typified by the Cahn-Hilliard equation. The method, based on the Hilbert expansion used in kinetic theory, besides its relative simplicity, leads to calculable higher order corrections to the interface motion. The present aim is to apply the Hilbert expansion approach, introduced in [3], to construct approximate solutions to (1).

Let Ω be a $d-$ dimensional torus having diameter much larger than the support of the interaction J. Write (1) as a gradient flow:

$$\frac{\partial}{\partial t}m = \nabla \cdot \left(\sigma(m)\nabla\left(\frac{\delta \mathcal{F}}{\delta m}\right)\right)$$

where $\sigma(m) = \beta(1-m^2)$ is the mobility,

$$\mathcal{F}(m) = \int_\Omega [f(m(x)) - f(m_\beta)]\mathrm{d}x + \frac{1}{4}\int_\Omega\int_\Omega J(x-y)[m(x)-m(y)]^2 \mathrm{d}x\mathrm{d}y,$$

and

$$f(m) = -\frac{1}{2}m^2 + \frac{1}{\beta}\left[\left(\frac{1+m}{2}\right)\ln\left(\frac{1+m}{2}\right) + \left(\frac{1-m}{2}\right)\ln\left(\frac{1-m}{2}\right)\right].$$

For $\beta > 1$, f is a symmetric double well potential on $[-1, 1]$. We denote the positive minimizer of f by m_β. Formally, one derives

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(m(t)) = -\int \left|\nabla\left(\frac{\delta\mathcal{F}}{\delta m}\right)\right|^2 \sigma(m(t))\mathrm{d}x$$

thus $\mathcal{F}$ is a Lyapunov function for (1). This suggests that the free energy should tend locally to one of the two minimizing values, $\pm m_\beta$, and that the interface between a region at $+m_\beta$ magnetization and a region at $-m_\beta$ magnetization should have a "profile" – in the direction orthogonal to the interface – that makes the transition from one local equilibrium to the other in a way that minimizes the free energy. This is indeed the case, as it has been shown in [1], [2]. The minimizers of the free energy $\pm m_\beta$ represent the "pure phases" of the system. However, unless the initial data m_0 happens to satisfy $\int_\Omega m_0(x)\mathrm{d}x = \pm m_\beta|\Omega|$, these "pure phases" cannot be reached because of the conservation law. Instead, what will eventually be produced is a region in which $m(x) \approx +m_\beta$, with $m(x) \approx -m_\beta$ in its complement, and with a smooth transition across its boundary. This is referred to a *phase segregation*, and the boundary is the *interface* between the two phases. If we "stand far enough back" from Ω, all we see is the interface, and we do not see any structure across the interface – the structure now being on an invisibly small scale. The evolution of m under (1) drives an evolution of the interface, and we wish to determine how it evolves. To see an evolution of the interface, one must wait a sufficiently long time. More specifically, let λ be a small parameter, and introduce new variables τ and ξ through $\tau = \lambda^3 t$, and $\xi = \lambda x$. Hence if $m(x,t)$ is a solution of (1), and we define $m^\lambda(\xi,\tau)$ by $m^\lambda(\xi,\tau) = m(x(\xi), t(\tau))$, we obtain

$$\frac{\partial}{\partial\tau}m^\lambda(\xi,\tau) = \frac{1}{\lambda}\nabla\cdot\left(\sigma(m^\lambda(\xi,\tau))\nabla\left[\frac{1}{\beta}\mathrm{arctanh}m^\lambda - (J_\lambda \star m^\lambda)\right]\right)(\xi,\tau) \tag{2}$$

where $J_\lambda(\xi) = \lambda^{-d}J(\lambda^{-1}\xi)$. Following Giacomin and Lebowitz [6], we will be studying solutions of the equation (2) in the limit as λ tends to zero. For the reasons indicated above, we shall consider initial data $m_0(\xi)$ with value $-m_\beta$ in the region bounded by a smooth closed curve Γ_0 in Ω, and $+m_\beta$ outside this region. We refer to such initial data as "sharp interface initial data". At later times t there will still be a fairly sharp interface between a region where $m(\xi,t) \approx +m_\beta$ and where $m(\xi,t) \approx -m_\beta$, centered on a smooth curve Γ_t. One might hope that for small values of λ, *all information about the evolution on $m(\xi,t)$ is contained in the evolution of the interface Γ_t*. This is indeed the case. Let $\mathcal{M}$ denote the set of all smooth simple closed curves in Ω. A vector field V on $\mathcal{M}$ is a functional associating to each Γ in $\mathcal{M}$ a function in $C^\infty(\Gamma)$. This function gives the normal velocity of each point on Γ, and thus describes a "flow" on $\mathcal{M}$. Formally

$$\frac{\mathrm{d}\Gamma_t}{\mathrm{d}t} = V(\Gamma_t)\ . \tag{3}$$

Now, given a flow on $\mathcal{M}$, we can produce an evolution in $C^\infty(\Omega)$ through the following device: Let m be any function from $\mathcal{M}$ to $C^\infty(\Omega)$. We can then define a time dependent function on Ω, $m(\xi,t)$, through $m(\xi,t) = m(\Gamma_t)(\xi)$. Notice that

time dependence in $m(\xi, t)$ enters only through the evolution of Γ_t. If, for small λ and sharp interface initial data, all of the information about the evolution of solutions of (2) were contained in the motion of the interface, then one might hope to find a vector field V on $\mathcal{M}$ governing the evolution of the interface, and a function m from $\mathcal{M}$ to $C^\infty(\Omega)$ so that (3) defines the corresponding solution of (2). The following is the basic ansatz for our construction relating an asymptotic expansion for a flow of curves in Ω to an asymptotic expansion for an evolution of functions in Ω.

Ansatz. *Let $V_0, V_1, V_2, \ldots$ be a sequence of vector fields on $\mathcal{M}$. For any given initial interface Γ_0 in $\mathcal{M}$, and all $N > 0$, let $\Gamma_t^{(N)}$ be the solution of*

$$\frac{\mathrm{d}\Gamma_t^{(N)}}{\mathrm{d}t} = \left[\sum_{j=0}^{N-1} \lambda^j V_j\right]\left(\Gamma_t^{(N)}\right) \qquad \text{with} \qquad \Gamma_0^{(N)} = \Gamma_0. \tag{4}$$

Let $m_0, m_1, m_2, \ldots$ be functions from $\mathcal{M}$ to $C^\infty(\Omega)$ defined as

$$m^{(N)}(\xi, t) = \sum_{j=0}^{N} \lambda^j m_j(\xi, \Gamma_t^{(N)}) \ .$$

Theorem. *For any $N > 1$ there are vector fields V_j, $j = 0, ..., (N-1)$ on $\mathcal{M}$ and functions m_j, $j = 0, ..., N$ from $\mathcal{M}$ to $C^\infty(\Omega)$ as prescribed in the ansatz having the following properties: Let T denote the lifetime of the solution of (4) in $\mathcal{M}$. Then there is a constant C_N so that for all $t < T$,*

$$\frac{\partial}{\partial t} m^{(N)} = \nabla \cdot \left(\sigma(m^{(N)}) \nabla \left(\frac{1}{\lambda}\left[\frac{1}{\beta} arctanh m^{(N)} - (J_\lambda \star m^{(N)})\right] + R^{(N)}\right)\right)$$

where

$$\sup_{\xi \in \Omega, t \in [0,T]} \left|R^{(N)}(\xi, t)\right| \leq C_N \lambda^{N-1} \ .$$

Finally the sequences of vector fields and functions are essentially uniquely determined: Given V_j for $j < k$, then V_k is determined up to $\mathcal{O}(\lambda^{k+1})$, and similarly given m_j for $j < k$, then m_k is determined up to $\mathcal{O}(\lambda^{k+1})$.

Giacomin and Lebowitz [5] by a formal analysis, discovered that in leading order, the evolution of the interface should be governed by the Mullins–Sekerka flow. Naturally enough, the corresponding vector field is the fist term, V_0, in our expansion in (4).

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An FKG type inequality for certain conditional measures

Agoston Pisztora

We consider a collection of binary 0-1 valued random variables $(X_e)_{e\in E}$ indexed by a finite set E. The corresponding probability space is $\Omega = \{0,1\}^E$ and $\omega \in \Omega$ is called a configuration. The joint distribution of the variables is denoted by P. Ω has a natural partial order: $\omega' \geq \omega$ iff $\omega'_e \geq \omega_e$ for every $e \in E$. A random variable $f : \Omega \to R$ is called increasing if $f(\omega') \geq f(\omega)$ for every pair $\omega' \geq \omega$. An event is increasing if its characteristic function is increasing. The FKG-inequality [2] guarantees non-negative correlations between increasing random variables whenever the so-called lattice condition is satisfied:

$$P(\omega \vee \omega')P(\omega \wedge \omega') \geq P(\omega)P(\omega')$$

where the min and max operations are performed coordinatewise. This condititon is easily verified for product measures. The FKG-inequality for events can be stated as follows: if $A, B \subset \Omega$ are increasing then $P(A|B) \geq P(A)$ (provided $P(B) \neq 0$). Heuristically this is understood as follows: The occurrence of B guarantees the occurrence of some 1-s (unless $B = \Omega$) which will make it easier for A to occur. By using the same argument one is tempted to believe the if A, B, C are all increasing events, then

$$P(A|B \cap C) \geq P(A|C) \tag{1}$$

However, this inequality turns out to be false in general as was observed by van den Berg and Kahn [1]. They provided a counterexample where A, B, C are connection events which we next define. We equip the index set with a geometric structure by interpreting the set E as the edge set of a graph $G = (V, E)$. The edge-configurations give rise to random subgraphs induced by the *open* edges (i.e. $X_e = 1$) only. For given subsets of vertices $S, T \subset V$ we define the *connection event* $\{S \leftrightarrow T\} \subset \Omega$ if there is a sequence of neighboring open edges linking some vertex

in S with another one in T. The complement of this event is denoted by $\{S \not\leftrightarrow T\}$ and is called a *disconnection event*. In [1] a surprising inequlity has been proved. If P is a product measure, $A = \{S \leftrightarrow T\},\ B = \{S \leftrightarrow U\},\ C = \{S \not\leftrightarrow Z\}$, where $S, T, U, Z \subset V$, then (1) is true. Note that the primary conditioning event C is a disconnection event, in particular it is decreasing.

The inequality (1) of van den Berg and Kahn is surprising but it is very specific and leaves a lot of questions open. Is this inequality specific to product measures (like the van den Berg-Kesten inequality)? Is it valid for connection events only? Why does (1) hold for disconnection event but not for a connection event?

By trying to answer these and other questions we obtained an FKG-type inequlity which in some aspects considerably generalizes (1). Let $Z \subset V$ be a fixed set of vertices of the graph G. We denote by C_z the edge-cluster of Z, i.e., the collection of open edges connected (by open edges) to some vertex in Z. If f is an increasing function (random variable) on Ω, we set $\tilde{f}(\omega) = f(\tilde{\omega})$, where $\tilde{\omega}_e = \omega_e$ if $e \notin C_z$ and $\tilde{\omega}_e = 0$ otherwise. Similarly, $\hat{f}(\omega) = f(\hat{\omega})$, where $\hat{\omega}_e = \omega_e$ if $e \in C_z$ and 0 otherwise. Note that $\tilde{f}$ 'senses' increasing information *off* C_z whereas $\hat{f}$ measures only what happens *on* the cluster C_z. For instance, if $f = 1_{\{a \leftrightarrow b\}}$ then

$$\tilde{f} = 1_{\{a \leftrightarrow b\}}\, 1_{\{a \leftrightarrow Z\}} \quad \text{and} \quad \hat{f} = 1_{\{a \leftrightarrow b \leftrightarrow Z\}}$$

or, if N is the number of open bonds then $\tilde{N}$ is the number of open bonds off C_z and $\hat{N}$ counts the open bonds in C_z. Note that even though f is increasing, $\tilde{f}$ is not monotone (neither increasing nor decreasing.)

Finally let us recall the definition of random cluster (or FK-percolation) measure Φ. For parameters $q > 0$ and $(p_e)_{e \in E}$

$$\Phi(\omega) = \frac{1}{Z_G}\, q^{cl(\omega)} \prod_{e: X_e(\omega)=1} p_e \prod_{e: X_e(\omega)=0} (1 - p_e)$$

where $cl(\omega)$ denotes the number of clusters in the configuration ω and Z_G is the normalizing constant.

Theorem. *Let D be a disconnection event of nonzero probability (D might also be Ω). If f, g are increasing random variables then both pairs $(\tilde{f}, \tilde{g})$ and $(\hat{f}, \hat{g})$ are positively correlated with respect to the (conditional) measure $\Phi(\cdot\,|D)$.*

The theorem can be generalized in various ways, for instance the cluster C_z can be replaced by more general random sets. Analogous statemets can be formulated for Ising-Potts models.

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Existence of weak solutions to the Mullins-Sekerka flow

Matthias Röger

The Mullins-Sekerka flow describes phase transitions in materials with negligible specific heat. Surface tension effects are included by imposing a geometric condition an the phase boundary. Luckhaus and Sturzenhecker (see [1]) gave a time-discrete approximation scheme and proved convergence under an additional condition on the approximations, excluding cancellation of parts of the phase boundaries in the limit. We use techniques from Geometric Measure Theory to give a general existence result.

Let the partitioning of a given body $\Omega \subset \mathbb{R}^3$ into a liquid and a solid phase, and the temperature distribution inside the body be described by functions

$$\begin{aligned} \mathcal{X} : (0,T) \times \Omega &\to \{0,1\}, \\ u : (0,T) \times \Omega &\to \mathbb{R}, \end{aligned}$$

where $(0,T)$ is a given time interval. The phase interface at time t is given as the common boundary of the "liquid" phase $\{\mathcal{X}(t,.) = 1\}$ and the "solid phase" $\{\mathcal{X}(t,.) = 0\}$. The Mullins-Sekerka flow consists of an energy balance equation,

$$\partial_t \mathcal{X} = \Delta u + f, \tag{1}$$

and the Gibbs-Thomson condition on the phase interface,

$$H(t,.) = u(t,.). \tag{2}$$

Here f denotes a given heat source and $H(t,.)$ the mean curvature of the phase interface, which we take positive for convex liquid phases.

Our main result is stated in the following Theorem (for simplicity we have not formulated initial and boundary conditions).

Theorem. *There exists functions $\mathcal{X} \in L^\infty(0,T;H^{1,2}(\Omega))$, $u \in L^2(0,T;H^{1,2}(\Omega))$ satisfying* (1) *in the sense of distributions and the Gibbs-Thomson law in the following sense: For almost all $t \in (0,T)$ a generalized mean curvature $H(t)$, as defined below, of $\partial^*\{\mathcal{X}(t,.) = 1\}$ exists and $\mathcal{H}^2$-almost everywhere on $\partial^*\{\mathcal{X}(t,.) = 1\}$ equation* (2) *holds.*

In [1] an implicit time-discretization of (1), (2) is introduced, using the gradient flow structure of the problem. The approximate solutions satisfy a Gibbs-Thomson law in a formulation which expresses the first variation of the Perimeter functional for characteristic functions of bounded variation. Under the assumption that the total surface area of the approximate phase interfaces is conserved, convergence of approximate Gibbs-Thomson within the BV-formulation is shown in [1].

In general parts of the phase interfaces can cancel in the limit, cusp-like singularities and "hidden boundaries" may occur. Thus convergence of approximate in Gibbs-Thomson laws cannot be expected in the BV-formulation and a suitable generalization is needed. We follow an idea of Schätzle and consider the limit

of the surface measures of approximate phase interfaces. In [4] a convergence result for approximate Gibbs-Thomson laws is derived. Under suitable assumptions, the limit of the surface measures yields an integral varifold which completes the phase interface, given as reduced boundary of a function of finite perimeter. This varifold has bounded first variation and a mean curvature of a certain integrability. In our time dependent situation, for different limit points of the surface measures an identification of their mean curvature on the phase interfaces is crucial. This result was proved in [3] and justifies a notion of mean curvature for quite general phase interfaces.

Proposition. *Let $\mathcal{X} \in BV(\Omega; \{0;1\})$. Assume that there is an integral $(n-1)$-varifold μ in Ω, with bounded first variation and*

$$\partial^* E \subset spt(\mu),$$

$$\vec{H}_\mu \in L^s_{loc}(\mu),\ s > n-1,\ s \geq 2.$$

Then the mean curvature of μ on $\partial^*\{\mathcal{X} = 1\}$ is entirely determined by $\mathcal{X}$ in the sense that

$$H := \vec{H}_\mu \cdot \frac{\nabla \mathcal{X}}{|\nabla \mathcal{X}|}$$

is equal for different completions μ as above. We call H the generalized mean curvature of $\partial^*\{\mathcal{X} = 1\}$.

To prove our existence result we combine the last proposition and [4] to identify also the first variations of different limit points of the surface measures. With arguments from [2] and compactness results derived in [1] we finally show the convergence to correct solutions of the problem.

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High Pressure Phase Transitions

Wilfried Schranz

In order to describe the thermodynamic properties of materials the knowledge of the "equation of state" (EOS) is essential [1,2]. In the earth interior structural phase transitions occur at very high temperatures and pressures. Some of the most prominent examples are the pressure induced phase transformations in Olivin

$(Mg_{1-x}Fe_x)_2SiO_4$ in the upper mantle or the solid-liquid phase transition of iron at about 6000 K and 330 GPa in the earth core [3]. Our understanding of materials at ultrahigh pressures has substantially increased due to developments in experimental methods, especially the diamond anvil cell.

In the presence of pressure induced phase transformations elastic anomalies are reflected through nonlinear variations of the lattice parameters and the corresponding compressibilities [4,5]. Presently in many phenomenological descriptions of high pressure data it is standard to describe the system in the different phases by seperate EOS with corresponding EOS parameters, which are not related to each other [6,7]. Althoug this method works in many cases it has the disadvantage to provide no insight into the mechanism of the phase transformation. Moreover one can hardly use the obtained parameters for calculation of other thermodynamic properties like specific heat, soft mode, etc. as a function of pressure.

To overcome these problems we have constructed a thermodynamic theory which is based on a Landau type free energy expansion in terms of the order parameter η and the strains ϵ_{ij}, and includes the order parameter part $F(\eta)$, the order parameter- strain coupling $F(\eta_{ij}, \epsilon)$ and the elastic part $F(\epsilon_{ij})$ of the free energy [8]. At extremely high pressures one faces two different types of nonlinearities:

(a) Geometric nonlinearities appear due to the fact, that for high deformations the strain tensor cannot be longer treated as infinitesimal, but one has to deal with finite strains [9].
(b) Physical nonlinearities appear as a consequence of high pressures and show up e.g. in a nonlinear pressure dependence of the volume, i.e. $V(P)$.

Usually $V(P)$ is fitted to nonlinear EOS of various kind, which are known in the literature as "Murnaghan-, Birch Murnaghan-, Vinet-, etc. EOS" [3]. For cubic systems it is trivial to find the pressure dependence of the axies from a given $V(P)$, i.e. to calculate the third root. For other symmetries this is a hard problem. We found expressions for the strains or the lattice parameters a, b, c as a function of hydrostatic pressure, which yield $a(P) \cdot b(P) \cdot c(P) = V(P)$ for tetragonal, and orthorhombic systems [8]. With these expressions we could calculate the nonlinear pure elastic free energy. Coupling these strains to the order parameters we have also constructed the Landau free energy to describe high pressure phase transitions.

Compared to the heuristic engineering proceedure using several EOSs a thermodynamic model represents a significant improvement, as it allows to relate different measurable quantities such as unit cell volume, compressibility, specific heat, soft mode frequencies, etc. via a pressure dependent order parameter to each other in a systematic way.

At present the theory works for cubic, tetragonal and orthorhombic systems and for phase transitions that are of the group-subgroup type. An improvement of the theory to account for phase transitions between other crystal systems and especially to describe pressure induced phase transitions which are not of the group-subgroup type is in progress.

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On phase field modelling of alloy solidification

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(joint work with H. Garcke and B. Nestler)

Solidification of alloys involves the formation of microstructures which essentially influence the properties and quality of castings. In order to describe such growth phenomena we have been developing a general model which allows for an arbitrary number of components in the alloy. It is based on a phase-field formulation to handle the moving phase boundaries in such a way that an arbitrary number of phases can be considered.

During the evolution, energy and mass are conserved and a local entropy inequality is satisfied. The model can easily be fit to arbitrary materials by choosing appropriate bulk free energies of the possible phases and suitable anisotropies for the phase boundaries and by inserting physical parameters like diffusivities, latent heats, and surface tensions. Besides, in the sharp interface limit if the diffuse interface thickness tends to zero, a classical model with moving phase boundaries is recovered. A full description can be found in [1].

The model is based on an entropy functional. The entropy density consists of a bulk part $s(e, c, \phi)$ and a surface part $\varepsilon a(\phi, \nabla\phi) + \frac{1}{\varepsilon} w(\phi)$. s depends on the internal energy density e, the volume fractions c_i of the N components and phase-field variables ϕ_α, each one describing the presence of the corresponding phase α. The surface terms only depend on the phase-field variables. w is some multi well potential with absolute minima in the points $e_\alpha = (\delta_{\alpha\beta})_{\beta=1}^{M} \in \mathbb{R}^M$ which correspond to the pure phases. a is some gradient term modelling surface tension

effects including anisotropy. The evolution is given by balance equations for mass and energy of the form

$$\partial_t e = -\nabla \cdot J_0, \qquad \partial_t c_i = -\nabla \cdot J_i, \quad 1 \le i \le N, \tag{1}$$

where the fluxes are postulated to be linear combinations of the thermodynamical forces. The corresponding potentials are given by $\frac{\partial s}{\partial e} = \frac{1}{T}$ and $\frac{\partial s}{\partial c_i} = \frac{-\mu_i}{T}$, T being the temperature and μ_i being the chemical potential of component i. We will write $u = (\frac{-1}{T}, \frac{\mu_1}{T}, \dots, \frac{\mu_N}{T})$, then $J_i = \sum_{j=0}^{N} L_{ij}(u,\phi)\nabla(-u_j)$, $0 \le i \le N$. The evolution of the phase-field variables is given by a gradient flow of the entropy,

$$\varepsilon\omega(\phi, \nabla\phi)\partial_t\phi = \frac{\delta S}{\delta \phi} - \lambda \tag{2}$$

with some possibly anisotropic kinetic coefficient ω. We refer to [2] for possible choices of the occuring functions.

The length scale ε corresponds to the characteristic interface thickness. In the limit as $\varepsilon \to 0$ (the sharp interface limit) a classical model with moving boundaries is recovered to first order in ε. The domain is divided into regions occupied by the pure phases. There, balance equations for e and c are satisfied. On the moving boundaries separating the phases, temperature and generalized chemical potential differences are continuous and jump conditions for the conserved quantities hold. The motion of the boundaries is coupled to the thermodynamical quantities by a Gibbs-Thomson condition in such a way that local entropy production is nonnegative.

As in numerical simulations the diffuse interface has to be resolved by the grid involving restrictions for the time step one is interested in a better approximation. In [3, 4] results for an approximation to second order in ε have been presented. They could be generalized to an arbitrary number of conserved quantities; the case of multiple phases is still an open problem. Based on the method of formally matched asymptotic expansions, a correction problem to order ε^1 is derived. Defining a small correction to the kinetic coefficient ω, functions identically zero solve this correction problem. In numerical simulation, second order convergence could indeed be observed when the correction term was taken into account.

Defining the reduced grand canonical potential ψ as the Legendre transformed of the entropy density with respect to the conserved quantities (e, c) (see [5]) and considering (u, ϕ) as the independent variables we can write down the governing set of equations in terms of ψ and derivatives,

$$\partial_t \psi_{,u_i}(u,\phi) = \nabla \cdot \sum_{j=0}^{N} L_{ij}\nabla u_j, \tag{3}$$

$$\varepsilon\omega\, \partial_t \phi_\alpha = \varepsilon\nabla \cdot a_{,\nabla\phi_\alpha} - \varepsilon a_{,\phi_\alpha} - \tfrac{1}{\varepsilon} w_{,\phi_\alpha} + \psi_{,\phi_\alpha}(u,\phi) - \lambda. \tag{4}$$

Existence and uniqueness of a weak solution of this system of parabolic equations can be shown under appropriate growth and structural conditions on ψ. To relax the assumptions, the application of results in [6, 7] is planned.

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Crystallization in 2 dimensions

Florian Theil

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

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

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

Theorem A (Asymptotic behaviour of the ground state energy per particle). *Let $d = 2$. There exists a constant $a > 0$ such that for all $V \in C^2(0, \infty)$ with the properties $V(1) = -1$, $\lim_{r\to\infty} V(r) = 0$ and*

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

the ground state energy has the following asymptotic behavior

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

The renormalized potential V_R, which is defined by

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

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

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

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

Theorem B (Ground states). *Let the assumptions of Theorem A be satisfied, $\mathcal{A} \subset A_2$ be an arbitrary bounded subset and $y_{\min}$ be a ground state of the modified energy*

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

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

Previously Radin obtained in [1] similar results for a specific choice of V. In the discussion several interesting point have been raised:

(1) Is it possible to define pressure by considing the constrained minimization $y(x) \in \sqrt{N}\Omega$ where $\Omega \subset \mathbb{R}^2$ is a bounded open set? Intuitively one would expect that the ground state energy per particle is given by

$$\min_{y \in \Omega^N} \tfrac{1}{N} E(y) = V_R^{**}\left(\sqrt{\tfrac{2}{\sqrt{3}}\mathrm{meas}(\Omega)}\right),$$

where V_R^{**} is the convexification of V_R.

(2) An application of the methods developed so far might also lead to a rigorous analysis of the Wigner-crystal where $V(r) = \frac{1}{r}$ is the Coulomb-interaction enery between electrons. For large densities it would be be necessary to work with a quantum mechanical version of the pair energy E.

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Dynamical problems with nonconvex energies as a model of damage in materials

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(joint work with Marc Oliver Rieger)

Young measures have been successfully applied to various mathematical problems in material science. Most notably, they are an appropriate tool to capture the formation of microstructure arising in problems of martensitic phase transitions. This approach has been pioneered by Ball and James [2]. There, Young measures describe the oscillations in microstructured materials arising from a nonconvex free energy density.

Though variational methods have turned out to be tremendously successful for the analysis of problems with nonconvex energy densities, an inherent difficulty is that the traditional variation approach gives the global minimiser, which may be unphysical. For fracture, Truskinovsky pointed out [7] that sublinear functionals like $\int \log\left(1+|u_x|^2\right)$ have a global minimiser with zero energy if the initial configuration is only stretched infinitesimally. That is, an elastic bar described by this model would break instantaneously if the energy were to obtain its *global* minimum. A natural strategy is therefore to search for *local* minimisers. To this aim, the concept of a quasi-static limit of Young measure gradient flows with respect to a regularized Wasserstein metric has been introduced [5].

We study the evolution of Young measures by means of a discretized gradient flow, where the energy density is sublinear. To be specific, we may assume the energy is convex in a neighbourhood of the origin and concave elsewhere.

A natural metric is given by the Wasserstein distance

$$d_W^p(\nu_1,\nu_2) := \frac{1}{2}\inf_{\mu}\left(\int_X\int_X |x-y|^p\, d\mu(x,y),\ \pi_1(\mu)=\nu_1,\ \pi_2(\mu)=\nu_2\right)^{\frac{1}{p}},$$

where $\pi_1(\mu)$ and $\pi_2(\mu)$, respectively, are the marginals, i.e., projections of the measure μ on $X\times X$ onto the first and second, respectively, component.

It turns out that the 1-Wasserstein metric provides a suitable scaling, while a p-Wasserstein metric with $p>1$ prohibits a "long-distance" mass transport between existing masses [5].

Problems in materials science often turn out to be asymmetric. For instance, nucleation and disappearance of a phase are not symmetric, since a nucleation barrier has to be overcome. We introduce a phenomenological asymmetric part to the metric. Namely, for two closed sets A and B, we define

$$d_H^+(A,B) := \sup_{a\in A}\inf_{b\in B} d(a,b). \tag{1}$$

This is "half" the Hausdorff distance

$$\max\left(\sup_{a\in A}\inf_{b\in B} d(a,b), \sup_{b\in B}\inf_{a\in A} d(a,b)\right);$$

we will consider time-discretized problems, where B will be the support of the measure at the previous time step, and A the support at the current time step.

This regularisation is clearly phenomenological. We will demonstrate that it nevertheless captures essential features of the dynamics. Specifically, the following variational problem will be studied. Given ν_0, define ν_j for $j\in\mathbb{N}$ as solution of

$$\inf_{\nu\in X}\int_\Omega\left[\frac{1}{2}d_W^1\left(\nu^j,\nu\right)^2+\frac{h}{\epsilon}\langle\Phi,\nu\rangle\right]\mathrm{d}x+\delta\sup_{x\in\Omega} d_H^+\left(\mathrm{supp}(\nu^j),\mathrm{supp}(\nu)\right) \tag{2}$$

(compare [4] for the connection to gradient flows without regularizing term). Here, X is the class of (gradient) Young measures (varifolds) with expectation value $F(t)$, i.e., $\int_\Omega \mathrm{d}\nu = F(t)$, where $F(t)$ is given.

Gradient flows in metric spaces have been thoroughly investigated [1]. An extension to flows in asymmetric metric spaces is ongoing [3].

Here, the focus is on qualitative properties of the solution to (2) in a one-dimensional situation. Suppose $\Omega := (0,1)$, and assume for simplicity that the energy Φ is convex in $B(0,1)$ (the ball with radius 1 centred at the origin), and concave elsewhere. For such an energy of Lennard-Jones type, stability properties can be shown for the space-homogeneous case, where where the measures are constant in x.

Proposition. If $F(t) = F < 1$, then the solution is stable everywhere in $(0,1)$. That means: $\nu^j(x)$ supported in $(0, 1-\eta)$ implies that $\nu(x)$ is supported in $(0, 1-\eta)$. If $F < 1$ and ν^j, ν^{j+1} are supported in $(0,1)$, then $\left(\text{supp}\left(\nu^{j+1}\right)\right)^{\text{conv}}$ is strictly contained in $\left(\text{supp}\left(\nu^{j}\right)\right)^{\text{conv}}$.

Corresponding results concerning the instability in the concave region will also be presented, as well as questions of existence. This allows for a discussion of how the mathematical model sketched above can serve as a description of damage occuring in a material.

A more detailed presentation will be published elsewhere [6].

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