# Mathematisches Forschungsinstitut Oberwolfach

# Phase Transitions

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ABSTRACT. Phase transitions are common phenomena which occur in many fields of material sciences. Models of phase transitions in diverse physical systems often lead to ill-posed mathematical problems whose solutions are characterized by oscillations, bifurcations and singularities. Random fluctuations and stochastic events also play an important role in determining the nature of the solutions.

## Introduction by the Organisers

Phase transitions are singular phenomena involving a collective behavior of many degrees of freedom. A wide range of mathematical models have been introduced: Their purpose stretches from capturing the essence of phase transitions (statistical mechanics) to quantitative prediction in engineering (continuum thermodynamics). Hydrodynamic limits with their mean-field models and large deviation principles form a bridge between these micro and mesoscopic descriptions. The presence of quenched disorder next to thermal fluctuations adds new phenomena — and complexity.

Not surprisingly, the mathematical methods are as diverse as the models: From combinatorics and probability theory to the calculus of variations and partial differential equations. Models of phase transitions typically cannot be dealt with by soft methods but require new tools. This workshop broadly brought together these mathematical communities of stochastics and analysis — along with a few physicists and engineers to discuss these problems.

Phase transitions in statistical mechanical setting have been discussed for lattice gradient models with non-convex potentials and for the six-vertex model with tilted boundary conditions. The phenomenon of Bose-Einstein condensation was addressed in the context of infinite cycles in spatial random permutations and on the level of large deviations for empirical measures for Brownian bridges and random integer partitions.

Phase transition from a theoretical engineering perspective have been mostly discussed in the context of shape memory alloys on the level of experimental observations and mesoscopic modeling. One talk related the magnitude of hysteresis not to the energy barrier for the formation of Martensite nuclei but to the size of preexisting nuclei; another talk investigated the influence of quenched disorder on this phase transition; a third talk proposed an artificial 2-d atomistic model tractable by numerical experiments.

Another important topic were mean field models and stochastic dynamics in the regime of phase segregation including corresponding large deviation principles for high-dimensional or spatially extended systems with many modes: nonlinear stability of fronts in non-local mean-field models, equilibrium pattern in mean-field models for diblock-copolymers, analysis of metastable behavior based on a computation of capacities for finer asymptotics beyond Wentzel-Freidlin theory, large deviation functionals for many-particle systems and spectral gap bounds for the stochastic Ising model, and logarithmic Sobolev inequalities for lattice models with continuous spin with applications to hydrodynamic limits.

Another topics was the analysis of the time-asymptotic behavior (coarsening, gelation) of coagulation models: For certain "collision" kernels, the analysis is fairly explicit, very elegant (and universal in the sense that it connects seemingly unrelated fields); for more generic kernels, subtle matched asymptotic expansions are required and new methods like a multi-scale maximal regularity theory for the linearized operator have to be developed. Related in spirit though not in techniques was a talk on Ostwald ripening for liquid droplets.

## Workshop: Phase Transitions

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# Abstracts

## Free energy of interacting Bosons

STEFAN ADAMS

(joint work with Andrea Collevecchio, Wolfgang König)

We consider $N$ bosons in a box in $\mathbb{R}^d$ with volume $N/\rho$ under the influence of a mutually repellent pair potential. The particle density $\rho \in (0, \infty)$ is kept fixed. Our main result is the identification of the limiting free energy, $f(\beta, \rho)$, at positive temperature $1/\beta$, in terms of an explicit variational formula, for any fixed $\rho$ if $\beta$ is sufficiently small, and for any fixed $\beta$ if $\rho$ is sufficiently small.

The thermodynamic equilibrium is described by the symmetrised trace of $e^{-\beta \mathcal{H}_N}$, where $\mathcal{H}_N$ denotes the corresponding Hamilton operator. The well-known Feynman-Kac formula reformulates this trace in terms of $N$ interacting Brownian bridges. Due to the symmetrisation, the bridges are organised in an ensemble of cycles of various lengths. The novelty of our approach is a description in terms of a marked Poisson point process whose marks are the cycles. This allows for an asymptotic analysis of the system via a large-deviations analysis of the stationary empirical field. The resulting variational formula ranges over random shift-invariant marked point fields and optimizes the sum of the interaction and the relative entropy with respect to the reference process.

## 1. THE MODEL

The main object is the following symmetrised sum of Brownian bridge expectations,

$$
(1) \quad
\begin{aligned}
Z_N^{(\mathrm{bc})}(\beta, \Lambda) = \frac{1}{N!} \sum_{\sigma \in \mathrm{Sym}_N} &\int_\Lambda \mathrm{d}x_1 \cdots \int_\Lambda \mathrm{d}x_N \\
&\times \bigotimes_{i=1}^N \mu_{x_i, x_{\sigma(i)}}^{(\mathrm{bc}, \beta)} \Big[ \exp\Big\{ - \sum_{1 \le i < j \le N} \int_0^\beta v(|B_s^{(i)} - B_s^{(j)}|) \, \mathrm{d}s \Big\} \Big].
\end{aligned}
$$

Here $\mu_{x,y}^{(\mathrm{bc}, \beta)}$ is the canonical Brownian bridge measure with boundary condition $\mathrm{bc} \in \{\emptyset, \mathrm{per}, \mathrm{Dir}\}$, time horizon $\beta > 0$ and initial point $x \in \Lambda$ and terminal point $y \in \Lambda$, and the sum is on permutations $\sigma \in \mathrm{Sym}_N$ of $1, \ldots, N$. The *interaction potential* $v \colon \mathbb{R} \to [0, \infty]$ is measurable, decays sufficiently fast at infinity and is possibly infinite close to the origin. Our precise assumptions on $v$ are in [1].

The boundary condition $\mathrm{bc} = \emptyset$ refers to the standard Brownian bridge, whereas for $\mathrm{bc} = \mathrm{Dir}$, the expectation is on those Brownian bridge paths which stay in $\Lambda$ over the time horizon $[0, \beta]$. In the case of periodic boundary condition, $\mathrm{bc} = \mathrm{per}$, we consider Brownian bridges on the torus. The quantity $Z_N^{(\mathrm{bc})}(\beta, \Lambda)$ is related to

the $N$-body Hamilton operator

$$\mathcal{H}_{N,\Lambda}^{(\mathrm{bc})} = -\sum_{i=1}^{N} \Delta_i^{(\mathrm{bc})} + \sum_{1 \le i < j \le N} v(|x_i - x_j|), \qquad \mathrm{bc} \in \{\mathrm{Dir}, \mathrm{per}\}$$

where $\Delta_i^{(\mathrm{bc})}$ stands for the Laplacian with bc boundary condition, i.e., it is equal to the trace of the projection of the operator $\exp\{-\beta \mathcal{H}_{N,\Lambda}^{(\mathrm{bc})}\}$ to the set of symmetric functions $(\mathbb{R}^d)^N \to \mathbb{R}$. The *limiting free energy* is defined as

$$f^{(\mathrm{bc})}(\beta, \rho) = -\frac{1}{\beta} \lim_{N \to \infty} \frac{1}{|\Lambda_{L_N}|} \log Z_N^{(\mathrm{bc})}(\beta, \Lambda_{L_N}),$$

where $|\Lambda_{L_N}| = N/\rho$, for any $\beta, \rho \in (0, \infty)$, any $d \ge 1$ and any $\mathrm{bc} \in \{\emptyset, \mathrm{per}, \mathrm{Dir}\}$. The existence of the thermodynamic limit under suitable assumptions on the interaction potential $v$ can be shown by standard methods, see, e.g., Ruelle 1969.

Since any permutation decomposes into cycles, and using the Markov property, the family of the $N$ bridges in (1) decomposes into cycles of various lengths. We conceive these initial-terminal sites as the points of a standard Poisson point process on $\mathbb{R}^d$ and the cycles as marks attached to these points. In Theorem 1 below we rewrite the partition function in terms of an expectation over a reference process, the marked Poisson point process $\omega_{\mathrm{P}}$. We only deal with empty boundary conditions here (the other cases are in [1]). The space of marks is then defined as $E = \bigcup_{k \in \mathbb{N}} \mathcal{C}_{k,\Lambda}$, where, for $k \in \mathbb{N}$, we denote by $\mathcal{C}_k$ the set of continuous functions $f \colon [0, k\beta] \to \mathbb{R}^d$ satisfying $f(0) = f(k\beta)$, equipped with the topology of uniform convergence. We sometimes call the marks *cycles*. By $\ell \colon E \to \mathbb{N}$ we denote the canonical map defined by $\ell(f) = k$ if $f \in \mathcal{C}_{k,\Lambda}$. We call $\ell(f)$ the *length* of $f \in E$. We consider spatial configurations that consist of a locally finite set $\xi \subset \mathbb{R}^d$ of particles, and to each particle $x \in \xi$ we attach a mark $f_x \in E$ satisfying $f_x(0) = x$. Hence, a configuration is described by the counting measure $\omega = \sum_{x \in \xi} \delta_{(x, f_x)}$.

**Reference process.** Consider on $\mathcal{C} = \mathcal{C}_1$ the canonical Brownian bridge measure $\mu_{x,y}^{(\beta)}$ which is a regular Borel measure on $\mathcal{C}$ with total mass equal to the Gaussian density $(4\pi\beta)^{-d/2} e^{-\frac{1}{4\beta}|x-y|^2}$. We write $\mathbb{P}_{x,y}^{(\beta)}$ for the normalized Brownian bridge measure on $\mathcal{C}$. Let $\omega_{\mathrm{P}} = \sum_{x \in \xi_{\mathrm{P}}} \delta_{(x, B_x)}$, be a Poisson point process on $\mathbb{R}^d \times E$ with intensity measure equal to $\nu$ whose projection onto $\mathbb{R}^d \times \mathcal{C}_k$ is equal to $\nu_k(\mathrm{d}x, \mathrm{d}f) = \frac{1}{k} \mathrm{Leb}(\mathrm{d}x) \otimes \mu_{x,x}^{(k\beta)}(\mathrm{d}f)$. Alternatively, we can conceive $\omega_{\mathrm{P}}$ as a marked Poisson point process on $\mathbb{R}^d$, based on some Poisson point process $\xi_{\mathrm{P}}$ on $\mathbb{R}^d$, and a family $(B_x)_{x \in \xi_{\mathrm{P}}}$ of i.i.d. marks, given $\xi_{\mathrm{P}}$. The intensity of $\xi_{\mathrm{P}}$ is $\overline{q} = \sum_{k \in \mathbb{N}} q_k$ with $q_k = \frac{1}{(4\pi\beta)^{d/2} k^{1+d/2}}$. Let $\mathtt{Q}$ denote the distribution of $\omega_{\mathrm{P}}$ and denote by $\mathtt{E}$ the corresponding expectation.

## 2. Results

We write $\langle P, F \rangle$ for the expectation of a function $F$ with respect to a probability measure $P$. Define the *Hamiltonian* $H_\Lambda \colon \Omega \to [0, \infty]$ by

$$H_\Lambda(\omega) = \sum_{x,y \in \xi \cap \Lambda} T_{x,y}(\omega), \qquad \text{where } \omega = \sum_{x \in \xi} \delta_{(x, f_x)} \in \Omega,$$

where we abbreviate

$$T_{x,y}(\omega) = \frac{1}{2} \sum_{i=0}^{\ell(f_x)-1} \sum_{j=0}^{\ell(f_y)-1} 1_{\{(x,i) \neq (y,j)\}} \int_0^\beta v(|f_x(i\beta + s) - f_y(j\beta + s)|) \, \mathrm{d}s.$$

The function $H_\Lambda(\omega)$ summarises the interaction between different marks of the point process and between different legs of the same mark; here we call the restriction of a mark $f_x$ to the interval $[i\beta, (i+1)\beta)]$ with $i \in \{0, \ldots, \ell(f_x) - 1\}$ a leg of the mark. Denote by $N_\Lambda^{(\ell)}(\omega) = \sum_{x \in \xi \cap \Lambda} \ell(f_x)$ the total length of the marks of the particles in $\Lambda \subset \mathbb{R}^d$.

**Theorem 1:** Fix $\beta \in (0, \infty)$. Let $v \colon [0, \infty) \to (-\infty, \infty]$ be measurable and bounded from below and let $\Lambda \subset \mathbb{R}^d$ be measurable with finite volume. Then, for any $N \in \mathbb{N}$, and $\mathrm{bc} \in \{\emptyset, \mathrm{per}, \mathrm{Dir}\}$,

$$(2) \qquad Z_N^{(\mathrm{bc})}(\beta, \Lambda) = \mathrm{e}^{|\Lambda| \overline{q}^{(\mathrm{bc})}} \mathbf{E}^{(\mathrm{bc})} \big[ \mathrm{e}^{-H_\Lambda(\omega_{\mathrm{P}})} 1\{N_\Lambda^{(\ell)}(\omega_{\mathrm{P}}) = N\} \big].$$

By $\mathcal{P}_\theta$ we denote the set of all shift-invariant probability measures on $\Omega$. The distribution $\mathtt{Q}$ of the above marked Poisson point reference process $\omega_{\mathrm{P}}$ belongs to $\mathcal{P}_\theta$. Define $\Phi_\beta(\omega) = \sum_{x \in \xi \cap U} \sum_{y \in \xi} T_{x,y}(\omega)$, where $U = [-1/2, 1/2]^d$ denotes the centred unit box.

For any $\beta, \rho \in (0, \infty)$, define

$$\chi^{(\leq)}(\beta, \rho) = \inf \left\{ I_\beta(P) + \langle P, \Phi_\beta \rangle \colon P \in \mathcal{P}_\theta, \langle P, N_U^{(\ell)} \rangle \leq \rho \right\},$$

$$\chi^{(=)}(\beta, \rho) = \inf \left\{ I_\beta(P) + \langle P, \Phi_\beta \rangle \colon P \in \mathcal{P}_\theta, \langle P, N_U^{(\ell)} \rangle = \rho \right\}.$$

These formulas range over shift-invariant marked processes $P$. They have three components: the entropic distance $I_\beta(P)$ between $P$ and the reference process $\mathtt{Q}$, the interaction term $\langle P, \Phi_\beta \rangle$ and the condition $\langle P, N_U^{(\ell)} \rangle = \rho$, respectively $\leq \rho$.

**Theorem 2:** Let $L_N = (\frac{N}{\rho})^{1/d}$, such that $\Lambda_{L_N}$ has volume $N/\rho$. Denote

$$\mathcal{D}_v = \left\{ (\beta, \rho) \in (0, \infty)^2 \colon (4\pi\beta)^{-d/2} \geq \rho \mathrm{e}^{\beta \rho \alpha(v)} \right\}.$$

Then, for any $\beta, \rho \in (0, \infty)$, and for $\mathrm{bc} \in \{\emptyset, \mathrm{Dir}, \mathrm{per}\}$,

$$\limsup_{N \to \infty} \frac{1}{|\Lambda_{L_N}|} \log Z_N^{(\mathrm{bc})}(\beta, \Lambda_{L_N}) \leq \frac{\zeta(1 + \frac{d}{2})}{(4\pi\beta)^{d/2}} - \chi^{(\leq)}(\beta, \rho),$$

$$\liminf_{N \to \infty} \frac{1}{|\Lambda_{L_N}|} \log Z_N^{(\mathrm{bc})}(\beta, \Lambda_{L_N}) \geq \frac{\zeta(1 + \frac{d}{2})}{(4\pi\beta)^{d/2}} - \begin{cases} \chi^{(\leq)}(\beta, \rho) & \text{if } (\beta, \rho) \in \mathcal{D}_v, \\ \chi^{(=)}(\beta, \rho) & \text{if } (\beta, \rho) \notin \mathcal{D}_v, \end{cases}$$

where $\zeta(m) = \sum_{k=1}^\infty k^{-m}$ denotes the Riemann zeta function.

## 3. Discussion

One of the most prominent open problem in mathematical physics is the understanding of *Bose-Einstein condensation (BEC)*, a phase transition in a mutually repellent many-particle system at positive, fixed particle density, if a sufficiently low temperature is reached. That is, a macroscopic part of the system condenses to a state which is highly correlated and coherent. The first experimental realization of BEC was only in 1995, and it has been awarded with a Nobel prize. In spite of an enormous research activity, this phase transition has withstood a mathematical proof yet. Only partial successes have been achieved, like the description of the free energy of the ideal, i.e., non-interacting, system (already contained in Bose's and Einstein's seminal paper in 1925) or the analysis of mean-field models or the analysis of dilute systems at vanishing temperature. However, the original problem for fixed positive particle density and temperature is still waiting for a promising attack. Not even a tractable formula for the limiting free energy was known yet that could serve as a basis for a proof of BEC.

It is conjectured by Feynman 1953 that BEC is signalled by the decisive appearance of a macroscopic amount of 'infinite' cycles, i.e., cycles whose lengths diverge with the number of particles. This phenomenon is also signalled by a loss of probability mass in the distribution of the 'finite' cycles. See [4] for proofs of this coincidence in the ideal Bose gas and some mean-field models.

Our methods are mainly probabilistic. The greatest adavantage of this approach is that it is amenable to a large-deviations analysis. The central object here is the *stationary empirical field* of the marked point process, which contains all relevant information and satisfies a large-deviations principle in the thermodynamic limit (see [2, 3]). Due to a lack of continuity in the functionals that describe the interaction and the mark lengths, the upper and lower bounds derived in this way, may differ in general. (At sufficiently high temperature, we overcome this problem by additional efforts and establish a formula for the limit.) This effect is not a technical drawback of the method, but lies at the heart of BEC.

In the proof of our lower bound of the free energy, we drop the interactions involving any cycle longer than a parameter $R$ that is eventually sent to infinity, and in our proof of the upper bound we even drop these cycles in the probability space. As a result, our two formulas register only 'finitely long' cycles. Their total macroscopic contribution is represented by the term $\langle P, N_U^{(\ell)} \rangle$, and the one of the 'infinitely long' cycles by the term $\rho - \langle P, N_U^{(\ell)} \rangle$. In this way, the long cycles are only indirectly present in our analysis: in terms of a 'loss of mass', the difference between the particle density $\rho$ and the total mass of short cycles. Physically speaking, this difference is the total mass of a *condensate* of the particles.

The values of the two formulas $\chi^{(\leq)}(\beta, \rho)$ and $\chi^{(=)}(\beta, \rho)$ differ if 'infinitely long' cycles do have some decisive contribution in the sense that the optimal point process(es) $P$ in $\chi^{(\leq)}(\beta, \rho)$ satisfies $\langle P, N_U^{(\ell)} \rangle < \rho$. We conjecture that the question whether or not the optimal $P$ in $\chi^{(\leq)}(\beta, \rho)$ has a loss of probability mass of infinitely long cycles is intimately related with the question whether or not $\chi^{(\leq)}(\beta, \rho) = \chi^{(=)}(\beta, \rho)$ and that this question is in turn decisively connected with the question

whether or not BEC appears. This is in accordance with Sütő's work [4]. The conjecture is that, for given $\beta$ and in $d \geq 3$, if $\rho$ is sufficiently small, then it is satisfied, and for sufficiently large $\rho$ it is not satisfied. The latter phase is conjectured to be the BEC phase. Future work will be devoted to an analysis of this question.

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## Gradient models with non-convex interactions

Marek Biskup

(joint work with R. Kotecký, H. Spohn)

A gradient field is a collection of real valued random variables indexed by vertices of an integer lattice $\phi := \{\phi_x \colon x \in \mathbb{Z}^d\}$. These variables are distributed according to the measure given by the formal expression

$$\frac{1}{Z} \exp\Big\{ -\sum_{\langle x,y \rangle} V(\phi_y - \phi_x) \Big\} \prod_x \mathrm{d}\phi_x,$$

where the sum goes over the nearest-neighbor pairs of vertices and $V \colon \mathbb{R} \to \mathbb{R}$ is the potential. We assume that the potential is even, continuous and bounded from below with a quadratic growth at infinity. In order for this expression to make sense, one either fixes the field to a prescribed boundary condition at the vertices outside a finite set, or considers the problem directly in infinite volume, where the above formula serves as a prescription for the conditional probability in finite volume given the configuration outside.

The model has a number of computable instances. First, in $d = 1$, the variables $\phi_{x+1} - \phi_x$ are independent and so the problem can be analyzed by means of large deviation theory. Also, in all $d \geq 1$, the case of purely quadratic $V$ is amenable to explicit computation because the measure is Gaussian. It turns out that a similar, albeit less explicit, description is available whenever $V$ is strictly convex.

In my presentation I will outline an approach to a specific model with non-convex $V$, that was developed in joint works with R. Kotecký and H. Spohn. We assume that $V$ admits the representation

$$\mathrm{e}^{-V(\eta)} = \int_{(0,\infty)} \rho(\mathrm{d}\kappa)\, \mathrm{e}^{-\frac{1}{2}\kappa\eta^2}$$

where $\rho$ is a measure that is compactly supported in $(0, \infty)$. It turns out that already the first non-trivial case,

$$\rho := p\delta_{\kappa_1} + (1-p)\delta_{\kappa_2}$$

exhibits departures from the picture established in the convex case. In particular, in $d = 2$ and for $\kappa_1 \gg \kappa_2 > 0$ there exists a value $p \in (0, 1)$ for which there are two infinite-volume measures of the above kind (for the same $V$) whose typical samples are leveled (i.e., have zero tilt) but exhibit different characteristic fluctuations [1]. Nonetheless, the large-scale fluctuation structure away from the (zero) mean is in all cases described by the Gaussian Free Field [2]. The model exhibits also other interesting features (e.g., lack of strict convexity of the surface tension) that are unheard of in the class of convex potentials [3].

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## Metastability in stochastic Allen-Cahn equations

ANTON BOVIER

(joint work with Florent Barret, Sylvie Méléard)

Metastability is in essence the dynamical equivalent of a first order phase transition in statistical mechanics. In equilibrium statistical mechanics, a first order phase transition is said to occur if a systems is very sensitive to the change of a parameter (resp. boundary conditions), in the sense that some extensive variables (e.g. density or magnetization) show a discontinuity as functions of some intensive variables (e.g. pressure or magnetic field). Dynamically, for a finite system, this fact manifests itself in that as the parameter is varied across the phase transition line, the system will remain a considerable (and mostly random) amount of time in the "wrong phase" before suddenly changing into the true equilibrium phase (i.e. the sensitive variable will change its value as a function of time with a random delay).

Metastability is a very widespread phenomenon that arises and a large variety of systems, both natural and artificial. In many instances, it has important effects that are crucial for the proper functioning of the system and there has been great interest in understanding metastability in quantitative terms over as least the last 100 years. Most metastable systems of practical relevance are many-body systems whose dynamics is very hard to analyze both analytically and numerically. This is particularly true with respect to metastability in view of the very long time scales that are involved.

One of the first *mathematical models* for metastability was proposed in 1940 by Hendrik Anthony Kramers [8]. It consists of the simple, one-dimensional diffusion equation

$$(1) \qquad dX_t = b(X_t)dt + \sqrt{2\epsilon}dB_t,$$

where $b(x) = -V'(x)$, with $V(x)$ a *double well potential*, i.e. a function with two local minima that tends to infinity at $\pm\infty$, and $B_t$ is Brownian motion.

Kramers' equation has become the paradigm of metastability. Kramers had been able to solve all interesting questions in the context of this model. In particular, he derived the so called *Kramers-formula* for the average transition time from one minimum to the other,

$$(2) \qquad \mathbb{E}_a \tau_b = \frac{2\pi}{\sqrt{V''(a)V''(z^*)}} \exp\left(\varepsilon^{-1}\left(V(z^*) - V(a)\right)\right)(1 + o(1)),$$

from a minimum $a$ via the maximum at $z^*$ to the minimum at $b$. Kramers also envisaged multi-dimensional versions of his equation, that he could not, however, solve rigorously. The multi-dimensional generalization of this formula is attributed to Eyring and called *Eyring-Kramers formula* (see also [12]). It reads

$$(3) \qquad \mathbb{E}_a \tau_b = \frac{2\pi\sqrt{\det\left(\nabla^2 F(z^*)\right)}}{\sqrt{|\lambda_0(z^*)\det\left(\nabla^2 F(a)\right)}} \exp\left(\varepsilon^{-1}\left(V(z^*) - V(a)\right)\right)(1 + o(1)),$$

Note that Eyring's so-called *reaction rate theory* [4] is based on quantum mechanical considerations and quite different from the classical theory of Kramers.

Their analysis started in earnest with the large deviation theory devised by Freidlin and Wentzell [7] in about 1970. They obtained a rigorous derivation of the exponential term in the multi-dimensional term (including situations where the drift is not a gradient). Rigorous proofs of the full Eyring-Kramers formula in the gradient case were given in [2, 3]. From the point of view of statistical mechanics models, infinite-dimensional version of the diffusion equation (1) arise naturally. The simples form is the stochastic *Allen-Cahn equation*,

$$(4) \qquad dX(x,t) = \frac{\gamma}{4\pi^2}\Delta X(x,t)dt - \nabla f(X(x,t))dt + \sqrt{2\varepsilon}dB(x,t)$$

where $B$ is space-time noise and $f(x)$ is a double-well potential, e.g. $f(x) = \frac{x^4}{4} - \frac{x^2}{2}$. This equation seems to have been first studied by Faris and Jona-Lasinio [5]. Freidlin [6] derived large deviation estimates for this equation. Martinelli et al. [10] derived the exponentiallity of the law of the transition time. Assuming the validity of the Eyring-Kramers formula in in the infinite-dimensional setting, Maier and Stein [9] obtained explicit expressions for the prefactor in the case of one spatial dimension. A discussion in general dimensions can be found in [11].

In a recent paper [1], we prove the validity of the Eyring-Kramers formula for the Allen-Cahn equation on the interval $[0, 1]$ for couplings $\gamma > 1$.

**Theorem.** *Let $\gamma \in (1, \infty)$. Then there exist $K < \infty$, independent of $N$, such that for all $N$ and $\varepsilon > 0$,*

$$N^{-1}\mathbb{E}_{I_-}\tau_{B_+} = c_N e^{\frac{1}{4\varepsilon}}\left(1 + R(N, \varepsilon)\right),$$

*where $|R(\varepsilon, N)| \leq K\sqrt{\varepsilon|\ln\varepsilon|^3}$.*

*In particular,*

$$\lim_{\varepsilon\downarrow 0}\lim_{N\uparrow\infty} N^{-1}e^{-\frac{1}{4\varepsilon}}\mathbb{E}_{I_-}\tau_{B_+} = \lim_{N\uparrow\infty}c_N \equiv V(\gamma)$$

*where*

$$V(\gamma) = V(\mu) = \prod_{k=1}^{+\infty}\Big[\frac{\mu k^2 - 1}{\mu k^2 + 2}\Big] < \infty.$$

The case of general coupling strength is only slightly more complicated and is being treated in a paper in preparation by F. Barret. The proof proceeds very much along the lines of [2].

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# Space-Time Large Deviations

## Nicolas Dirr

(joint work with  A. De Masi, G. Manzi, E. Presutti, D. Tsagkarogiannis, S. Adams, M. Peletier, J. Zimmer)

It is well known that statistical mechanics and the theory of large deviations are closely related. For example, the free energy $F_\beta(m)$, as a function of the magnetisation $m$ in a mean field Ising model, describes the exponential rate of probability of the empirical magnetisation being close to a value $m$. Here we look at stochastic processes, i.e. at empirical measures on both space and time.

## 1. Pattern formation for action functionals

We consider an Ising-Model with Kac-Potential and Glauber Dynamics, i.e. we define a process on the state space $\bar{\sigma} : \Lambda \subset \mathbb{Z} \to \{-1, 1\}$ by specifying the rate at which the random variables (spins) $\sigma(X), X \in \mathbb{Z}$ change their sign (i.e. flip): Given a compactly supported interaction kernel $J \geq 0$, we define at a point $X \in \mathbb{Z}$ a local mean field by the $J$-weighted average over a $\gamma^{-1}$- neighbourhood , where $\gamma > 0$ is a small parameter, i.e.

$$h_{eff}(X) = \sum_Y \gamma^d J(\gamma|X - Y|)\sigma(Y).$$

The dynamics (Glauber, i.e. non-conserved) is such that the flip rate depends on $\sigma(X)$ and $h_{eff}(X)$ in such a way that aligning with neighbours is preferred (ferromagnetic) and that the dynamics is reversible (for finite $\gamma$) with respect to the Gibbs measure associated with the Hamiltonian

$$H(\bar{\sigma}) := -\frac{1}{2} \sum_X \sigma(X) \sum_Y \gamma^d J(\gamma|X - Y|)\sigma(Y).$$

A coarse graining (averaging over boxes) introduces a new random variable

$$m^\gamma(X, t, \omega) := (\gamma^\alpha)^d \sum_{|Y-X|_\infty < \frac{1}{2}\gamma^{-\alpha}} \sigma(Y, t, \omega).$$

Under a space rescaling to a so-called mesoscopic scale, $x = \gamma X$, one can show (see [3]) that $m^\gamma$ converges in probability to a deterministic function $m$ which solves a nonlocal evolution equation, $\partial_t m = -m + \tanh(\beta J * m)$, where $*$ denotes convolution. The mesoscopic free energy of the "static" system decreases along trajectories.

We are interested in deviations from this deterministic limit on a so-called *diffusive scale*, where space is rescaled with $\varepsilon = \varepsilon(\gamma)$ and time with $\varepsilon^2$. More precisely, we consider a spatially non-constant stationary solution $\bar{m}$ of our deterministic evolution equation at time $t = 0$, and ask for the probability that we see a stationary solution translated by $\varepsilon^{-1}R$ at time $\varepsilon^{-2}T$. (These solutions, so called instantons, correspond to interfaces on the diffusive scale.) As they are stationary solutions of the limit equation, this probability vanishes, but the exponential rate can be described by a so-called action functional. The most likely way in which an unlikely event happens (or, in other words, with conditional probability 1, conditioned on

the event of seeing at time $\varepsilon^{-2}T$ the stationary solution shifted by $\varepsilon^{-1}R$) is obtained by minimising this action functional. It turns out that for high velocities $V = R/T$ on the diffusive scale it is favourable to $2n$ additional interfaces that travel with uniform velocity $V/(2n+1)$ instead of shifting the initial "interface" with uniform velocity $V$. The cost converges as $\varepsilon \to 0$ to

$$w_n(R,T) := n2\mathcal{F}(\bar{m}) + (2n+1)\left\{\frac{1}{\mu}\left(\frac{V}{2n+1}\right)^2 T\right\}$$

where $F(\bar{m})$ is the free energy of an "interface" and $\mu$ a constant called "mobility." Note that the functional has a static part containing a free energy and a dynamic part penalising the velocity. Results in this spirit have been obtained for a simplified action functional in [2], for an action functional connected to the Allen-Cahn equation by [6], [7], [8] and for the exact spin system described above by Dirr, Manzi and Tsagkarogiannis (in preparation).

## 2. Large Deviations and Gradient Flows in Wasserstein distance

With $N$ independent Brownian motions $X_i$, $i = 1, \ldots, N$, on $[0,1]$, we can associate a random probability measure, the *empirical measure*

$$\mu_N(t,\omega,dx) := \sum_{i=1}^{N} N^{-1}\delta_{X_i}(dx).$$

Then it is well known that $\mu_N(t) \rightharpoonup \rho(t)dx$, where $\rho$ is deterministic and solves the heat equation $\partial_t \rho(t,x) = \Delta\rho(t,x)$.

**Gradient Flows:** Jordan, Kinderlehrer and Otto, [4], showed that the heat equation is a gradient flow of the entropy functional $E(\rho) = \int \rho \log \rho \, dx$ with respect to the 2- Wasserstein distance as dissipation distance on the infinite dimensional manifold $\mathcal{X} = \mathcal{M}_1(\mathbb{R})$ of probability measures. In particular, the *time-discrete approximating sequence* $\{\rho^n\}$ defined by

$$\rho^n \in \operatorname{argmin}_{\rho\in\mathcal{X}} K_h(\rho\,;\rho^{n-1}), \ K_h(\rho\,;\rho^{n-1}) := \frac{1}{2h}d(\rho,\rho^{n-1})^2 + E(\rho) - E(\rho^{n-1}).$$

converges to a solution of the heat equation as the time-step $h \to 0$, when $d$ is the 2-Wasserstein distance.

We aim to address the following questions in the context of limits of particle systems:
Why is the choice of Wasserstein distance and entropy more "physical" for describing the heat equation as gradient flow than e.g the -$L^2$-distance and the Dirichlet energy? What is the physical meaning of Wasserstein distance in the context of particle systems? And does the functional $K_h(\rho\,;\rho^{n-1})$ have a meaning away from the minimiser?

**Connection to particle model** The following observation hints already at a strong relation of the 2-Wasserstein distance to particle systems: Kipnis and Olla, [5], found the large deviations rate functional for the deviations of the empirical

measure associated with many Brownian motions from the heat equation. This functional can (formally) be written as

$$I(\rho) = \int_0^T g_{\rho(t)}(\dot\rho + \nabla E, \dot\rho + \nabla E)\mathrm{d}t,$$

where $g$ is the metric on the infinite dimensional manifold $\mathcal{M}_1$ that gives rise to the Wasserstein distance, and $\nabla E$ is the gradient associated via the metric to the exterior derivative $dE$.

A yet stronger justification and answer to the third question is given by the fact that $K_h(\rho\,;\rho^{n-1})$ appears in a $\Gamma$-expansion of a large deviations rate functional for $N$ Brownian motions, $N \to \infty$ after a time step of length $h$, where first $N \to \infty$ and then $h \to 0$. The $\Gamma$-expansion is performed with respect to $h$. More precisely, the rate functional after a time step $h$ (conditional on starting from $\rho_0$) is

$$J_h(\rho\,;\rho_0) \quad := \quad \inf_{q\,:\,\pi_2 q = \rho_0,\,\pi_2 q = \rho} H(q\,|\,q_0).$$

$$H(q|p) \quad := \quad \int\limits_{\mathbb{R}\times\mathbb{R}} f(x,y)\log f(x,y)\mathrm{d}p((x,y)) \text{ if } q \ll p, f = \frac{\mathrm{d}q}{\mathrm{d}p}$$

where the relative entropy $H(q|p)$ (for measure on the Cartesian product) is infinite if $q$ is not absolutely continuous w.r.t. $p$.

Our main technical result is the $\Gamma$-**expansion**

$$J_h(\,\cdot\,;\rho_0) - \frac{1}{4h}d(\,\cdot\,,\rho_0)^2 \longrightarrow \frac{1}{2}E(\,\cdot\,) - \frac{1}{2}E(\rho_0).$$

w.r.t weak convergence of measures. Here again $d$ is the 2-Wasserstein distance and $E(\rho) = \int \rho \log(\rho)$.

So far, this result is restricted to measures with Lebesgue density uniformly close to a constant and for systems on a compact space interval.

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## Hysteresis of a many-particle system due to non-monotone constitutive behavior

WOLFGANG DREYER

(joint work with Clemens Guhlke, Michael Herrmann)

**Introduction.** We study the behavior of systems that can be described as ensembles of interconnected storage particles. Our examples concern the storage of lithium in many-particle electrodes of rechargeable lithium-ion batteries and the storage of air in a system of interconnected rubber balloons. We are particularly interested in those storage systems whose constituents exhibit non-monotone material behavior leading to transitions between two coexisting phases and to hysteresis. In the current study we consider the case that the time to approach equilibrium of a single storage particle is much smaller than the time for full charging of the ensemble. In this regime, the evolution of the probability to find a particle of the ensemble in a certain state may be described by a nonlocal conservation law of Fokker-Planck type. The resulting equation contains two parameters which control whether the ensemble transits the 2-phase region along a Maxwell line or along a hysteresis path, or whether the ensemble shows the same non-monotone behavior as its constituents.

**The general model.** We propose a general model of a storage system that consists of an ensemble of many interconnected storage particles. The thermodynamic state of a single storage particle is described by a single variable $\xi \in [a, b]$. Any particle of the ensemble is equipped with a double well free energy function $F(\xi)$, so that two coexisting phases are possible. The prescribed mean number $q(t)$ of stored molecules in a particle is represented by the mean value of a given strict monotone function $G(\xi)$. The statistical behavior of the ensemble is represented by a probability density $w(t, \xi) \geq 0$, whose initial- and boundary value problem reads

$$w(0, \xi) = w_0(\xi), \qquad v(t, a)w(t, a) = v(t, b)w(t, b) = 0,$$

(1)
$$\frac{\partial w(t, \xi)}{\partial t} + \frac{\partial v(t, \xi)w(t, \xi)}{\partial \xi} = 0,$$

$$\tau v(t, \xi) = \left( \Lambda(t)G'(\xi) - F'(\xi) \right) - \nu^2 \frac{\partial \log(w(t, \xi))}{\partial \xi} \ .$$

The problem is non-local and non-linear because the function $\Lambda(t)$ must be calculated from the side condition

(2)
$$q(t) = \int_a^b G(\xi)w(t, \xi)d\xi \ .$$

**Non-monotone constitutive behavior.** Next we will consider two different applications, that have the non-monotonicity of the crucial constitutive function in common. The first example concerns the charging-discharging process of a lithium-ion battery, where lithium atoms are reversibly stored on interstitial lattice sites of iron phosphate particles forming one of the two electrodes of the battery.

The chemical potential $\mu = F'(y)$ of the $Li_yFePO_4$ crystal, where $y \in \{0, 1\}$ is the lithium mole fraction of a single $FePO_4$ storage particle, has the non-monotone shape given in Figure 1. The generic function $G(\lambda)$ is the identity.
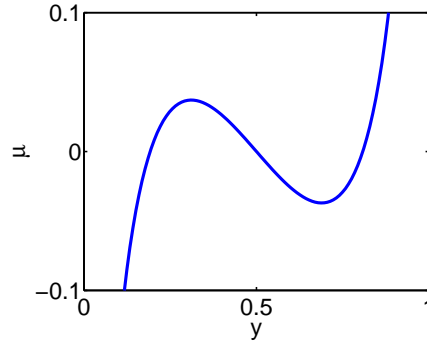


FIGURE 1. Chemical potential of a $Li_yFePO_4$ storage particle.

In the second examples we consider a system of interconnected rubber balloons that may serve to store air. In this case the statistical variable $\xi$ is the strain $\lambda = r/r_0$ of a single balloon, where $r$ and $r_0$ indicate the radii of the actual balloon and the undeformed balloon, respectively. The non-monotonicity here concerns the pressure difference across the membrane of a single balloon as a function of the strain, which qualitatively exhibits the same shape as the chemical potential of $Li_yFePO_4$. The generic function is related to the number $N(\lambda)$ of air molecules by $G(\lambda) = N(\lambda)/\bar{N}$, where $\bar{N}$ is the number of air molecules in the undeformed balloon.

**Configurational entropy.** The properties of solutions of the model are controlled by the two constant positive parameter $\tau$ and $\nu^2$. The parameter $\tau$ represents the relaxation time of the system and $\nu^2$ controls the influence of the configurational entropy. It describes interaction of the storage particles by exchange of Li atoms and air molecules, respectively. This interaction is important for low charging rates, where it leads to two peculiar phenomena. 1. The storage particles are not loaded at the same time, but according to the rule *one after the other*. 2. The phase transition leading to two coexisting phases does not happen within a single storage particle, rather it is a property of the many-particle ensemble. We observe particles with small filling, forming one phase, and particles with large filling, forming the second phase.

**Selected simulations for the many-particle electrode.** In this section we study a many-particle electrode of a rechargeable lithium-ion battery. We prescribe the history of loading-unloading processes by the filling degree $q(t)$ and solve the evolution equation for the probability density $w(t, y)$.

We solve the equation for $y \in [0, 1]$ and with boundary conditions $v(t, 0)w(t, 0) = v(t, 1)w(t, 1) = 0$. Initially we start the simulation in the 1-phase region, where the storage particles are Gaussian distributed around a small value, $q_0 = 0.1$, for

the initial filling degree, viz.

$$(3) \qquad w(0, y) = w_0(y) = \sqrt{\frac{\mu'(q_0)}{2\pi\nu^2}} \exp\left(-\frac{\mu'(q_0)}{2\nu^2}(y - q_0)^2\right).$$

In [2] we have performed simulations for 45 different values of $(\tau, \nu^2)$ but with the same loading-unloading path: At first we increase the filling degree $q$ linearly from $q = 0.1$ to $q = 0.9$ and afterwards we decrease it from $q = 0.9$ to $q = 0.1$. The time $t$ has been normalized by $|\dot{q}| = 1$, so the parameter $\tau = \tau_D/\tau_L$ gives the ratio between relaxation time $\tau_D$ of the storage system and loading time $\tau_L$. In particular, for fixed $\tau_D$ a small $\tau$ corresponds to a large loading time. The next Figure shows a typical evolution for parameter $\tau$ and $\nu^2$ so that a two phase region appears.
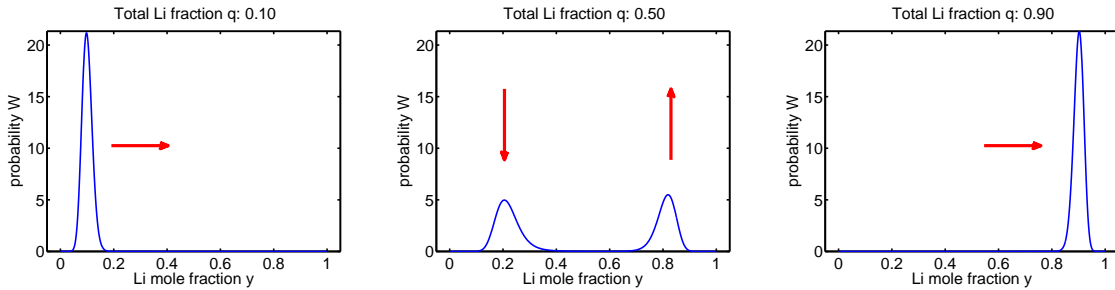


FIGURE 2. Evolution of the probability density for a loading process.

The loading-unloading process runs at the rate $\dot{q}$, where the total mole fraction $q(t)$ is linearly related to the total charge of the battery and the mean chemical potential

$$(4) \qquad \langle\mu\rangle(t) = \int_0^1 \mu(y)W(t, y)dy$$

is linearly related to the cell voltage. Figure 3 shows some examples.
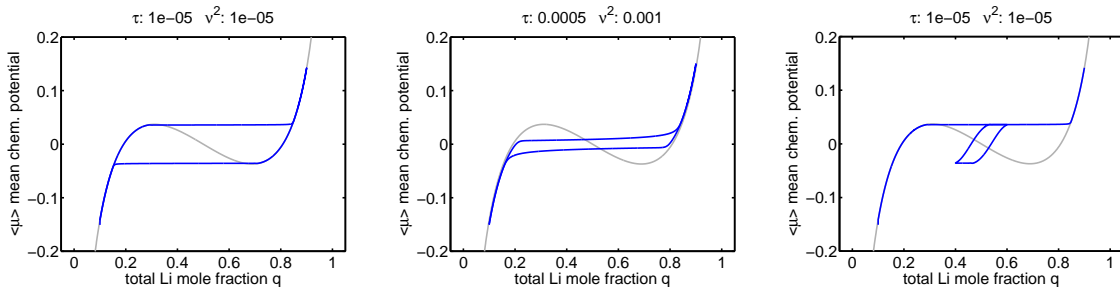


FIGURE 3. Hysteresis loops for various parameter and scenarios.

The location and the shape of the hysteresis is controlled by the two parameter $\tau$ and $\nu^2$. The details of the hysteresis curves can be quite involved but we observe three main cases:

(1) Case **A**: The probability density consists of a single pulse only, because there is not sufficient time to interchange molecules between the storage particles according to the configurational entropy effect. The mean chemical potential follows the chemical potential of a single particle.

(2) Case **B**: The configurational entropy is dominant and the storage system follows the Maxwell line. A hysteresis does not develop here.

(3) Case **C**: The deterministic evolution of the system and interchange of molecules due to the configurational entropy are of the same order. A maximal possible hysteresis is developed, see left diagram of Figure 3.

The diagram on the right hand side of Figure 3 concerns a different loading-unloading history that serves to demonstrate that it is possible to change between the loading and unloading plateaus without leaving the two-phase region.

**An experiment with rubber balloons.** Finally a system of interconnected rubber balloons serves to demonstrate the rule *one after the other* and to establish the phase separation. The sequence of snapshots in Figure 4 are generated for the analog loading-unloading path as above. Initially we observe only balloons with small filling. After a critical filling degree is reached, the transition to a second phase with large balloons sets in. In this period the balloons grow *one after the other* and we have a system of two coexisting phases with small and large balloons.
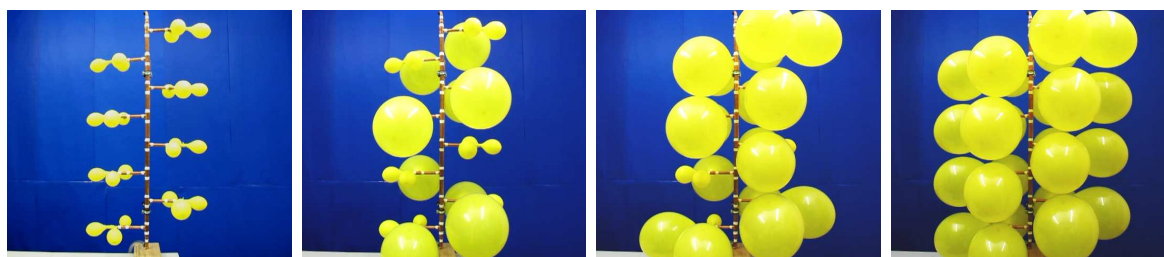


FIGURE 4. Four different states of interconnected rubber balloons during loading with air via the pressure vessel. From [2].

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## Microstructure formation and hysteresis in shape memory alloys

### Oliver Kastner

(joint work with Graeme Ackland)

Shape memory alloys (SMA) exhibit a number of features which are not easily explained by equilibrium thermodynamics, including hysteresis in the phase transformation and "reverse" shape memory in the high symmetry phase. Processing

can change these features: repeated cycling can "train" the reverse shape memory effect, while changing the amount of hysteresis and other functional properties. In the talk we present a molecular dynamics simulation study on this behaviour.

To simulate free evolutions of domain structures, atomic test assemblies must be sufficiently large and long computation times are required. Simulations of realistic 3D models therefore are limited by the computational ressources available. Therefore we employ a 2D Lennard-Jones model proven to represent a reliable qualitative model system for martensite/austenite transformations [1, 3, 4, 5]. We investigate the formation of microstructure and the evolution of defect structures in simulations of cyclic transformation/reverse transformation processes with this model. The simulations show that the transformation proceeds by non-diffusive nucleation and growth processes and produces distinct microstructure, see figure. Upon transformation, lattice defects are generated, which affect subsequent transformations and vary the potential energy landscape of the sample. If the sample is cycled through a series of forward/reverse transformations, the amount of defects in each phase accumulate. Defects act as nucleation sources for the transition. Moreover, the location of the defects can be preserved through the cycling, providing a memory of previous structures.

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## Hysteresis and phase transformations

Richard D. James

(joint work with J. Ball, C. Chu, R. Delville, S. Müller, N. Schryvers, V. Srivastava, J. Zhang)

Hysteresis refers to a phenomenon in phase transformations in which the transformation temperature on cooling is strictly lower than the transformation temperature on heating. It is considered to be part of the physical definition of a first-order phase transformation and thus its presence is ubiquitous. A plot of a typical property of the material vs. temperature exhibits a loop, called a *hysteresis loop*. Hysteresis also occurs during stress-induced or electromagnetic-field-induced transformation, exhibited as a loop in stress-strain space in the former case. While
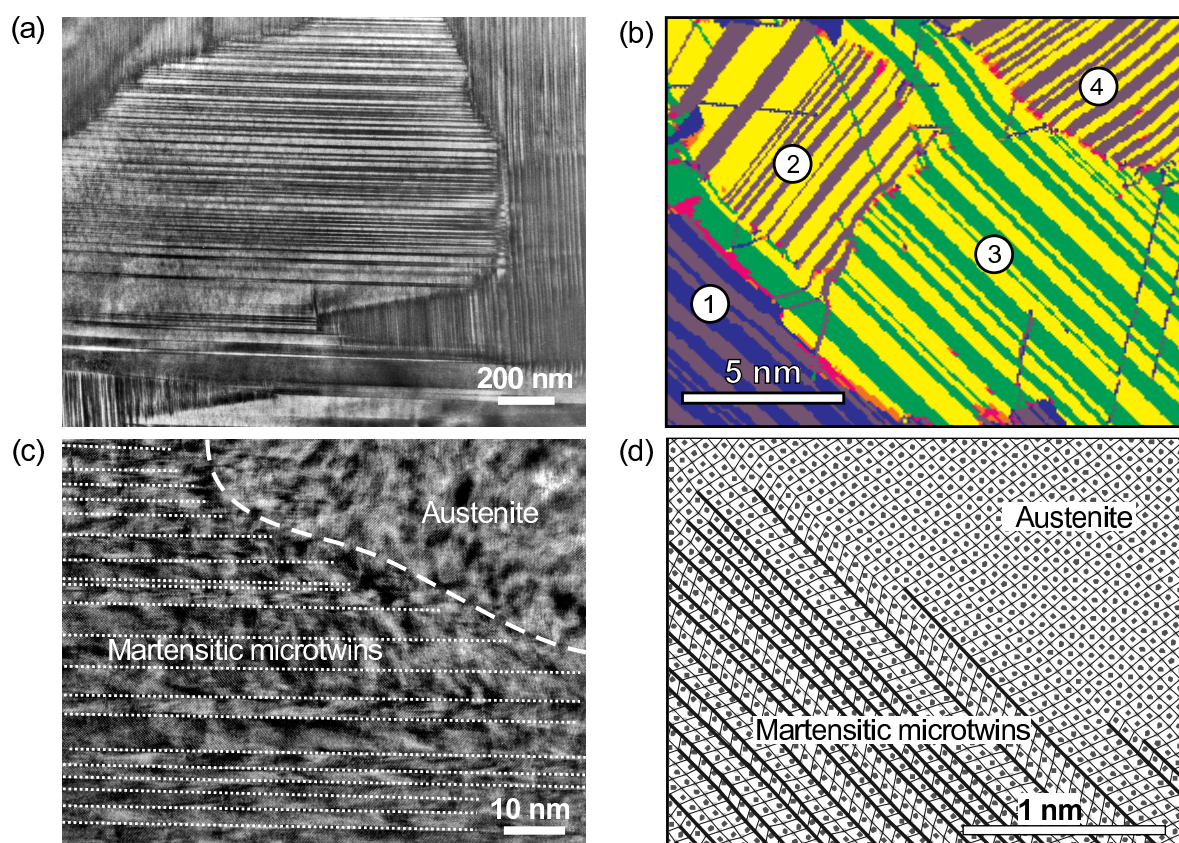
FIGURE 1. HRTEM images of NiAl (a,c) and simulated microstructures (b,d) in a binary 2D Lennard-Jones crystal. Colours indicate 4 variants of martensite present in the model which may nucleate on two perpendicular axes. In the MD, the model material exhibits martensite plates which are formed by compatible twin-variants. Plates which nucleate independently (① - ④) show incoherent, curved domain boundaries where growing into contact and dislocations are generated. The domain structure yielded by the 2D simulations is remarkably realistic-looking. Note no effort was spent to parameterise the model with respect to any real material, thus the characteristic length scales deviate by approximately one order of magnitude. HRTEM images courtesy D. Schryvers [6].

there are longstanding mathematical models such as the Preisach model that are designed to give hysteresis loops, they do not shed much light on the origins of hysteresis, and therefore do not give insight into ways of affecting or controlling it by modifying the material. In theoretical models hysteresis can often be related to dissipated energy, with larger loops associated to more wasted energy. These days, with the possibility of using transforming materials as energy conversion devices, the desire to reduce hysteresis is becoming an important societal problem.

Textbook descriptions of hysteresis typically relate its presence to either thermal activation or the pinning of interfaces by defects. People lean toward the latter for hard materials. Both of these areas have well-developed mathematical descriptions (resp., transition state theory, pinning models), but the connection with experiment is vague. For example, when people have tried to increase the number of pinning sites by increasing the density of defects in a crystal, they have seen a rounding of the loop but not much change in its size.

This lecture concerns a new idea for the origins of hysteresis that is primarily geometrical. It concerns the compatibility of the two phases. When transformations occur there is usually a change of the crystal structure and a change of lattice parameters. A crystal is usually described as a finite union of interpenetrating Bravais lattices in 3D, of the form $\cup_{j=1,...,n,\ \nu\in\mathbb{Z}^3}(\mathbf{c}_j + \sum_{i=1}^3 \nu^i \mathbf{e}_i)$. Using this description we can associate to each phase $n+3$ vectors, $\{\mathbf{c}_j^a; \mathbf{e}_i^a\}$ and $\{\mathbf{c}_j^m; \mathbf{e}_i^m\}$, the superscripts $a$ and $m$ denoting the two phases *austenite* and *martensite*[1]. The two sets of (linearly independent) vectors $\{\mathbf{e}_i^a; \mathbf{e}_i^m\}$ are related by an invertible linear transformation, $\mathbf{e}_i^m = \mathbf{A}\mathbf{e}_i^a, i = 1,2,3$. The thesis of the talk is that the size of the hysteresis loop in broad classes of crystalline materials that undergo diffusionless phase transformations is strongly related to the the middle eigenvalue $\lambda_2$ of $\mathbf{A}^T\mathbf{A}$, with the value $\lambda_2 = 1$ giving the minimum hysteresis [5, 3, 8, 4] .

The parameters $\mathbf{e}_i^{a,m}$ and therefore $\mathbf{A}$ can be changed by changing the composition of the material: this is particularly easy in metals, but it is also possible in oxides by suitable doping. (These are diffusionless transformations, so the composition of the material does not change upon transformation, but it can be altered when the crystal is originally made, for example, by melting together varying proportions of the individual elements that make up the alloy.) We present in the talk numerous cases [3, 8] in which the composition was tuned to make $\lambda_2 = 1$. Measured plots of the size of the hysteresis loop vs. $\lambda_2$ give a dramatic drop at $\lambda_2 = 1$, with an apparent singularity. With large numbers of alloys made by combinatorial synthesis methods [3, 7], the minimum hysteresis is smaller than the experimental error of its measurement [7]. In careful bulk synthesis methods in which composition is varied by $1/4\,\%$ increments, the minimum hysteresis is in the range $2-5°C$, otherwise independent of alloy in cases studied so far. It is common for the size of the hysteresis loop to change by a factor of 10 as $\lambda_2 \to 1$. The fact that people synthesized a great many alloys in the past and measured the hysteresis, but did not notice the connection with $\lambda_2 = 1$, is apparently owing to the singular nature of the drop: one has to be extremely close to $\lambda_2 = 1$ to see the dramatic effect.

In the talk a theory from [8] is presented for this effect. The idea is that the bulk and interfacial energy that is necessarily present near the interface between phases when $\lambda_2 \neq 1$ gives rise to an energy barrier. This energy barrier is calculated within the context of a rather strong ansatz for the structure of a growing nucleus of the new phase. Beginning in the high temperature austenite phase, this

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[1]The number $n$ can also depend on the phase.

barrier decreases as the temperature is lowered. But its height at a given value of temperature is dramatically dependent on $\lambda_2$.

This elementary theory gives a plot of the size of the hysteresis vs. $\lambda_2$ that is similar to the one measured in experiment [8]. However, it is pointed out in the lecture that this energy barrier apparently does not correspond to any known mathematical concept in the calculus of variations. That is, while it seems related to local minimizers, most closely to the concept of "hysteresis induced by incompatibility" studied earlier [1, 2], there is apparently no known definition[2] of local minimizer that would give the observed behavior of the hysteresis vs. $\lambda_2$. It is possible that the explanation for this behavior lies outside the realm of the calculus of variations and more in dynamics, or in models that explicitly account for defects[3]. The author believes, however, in the possibility of a relatively simple but general quantitative explanation based on some version of metastability in the calculus of variations, in which defects are not explicitly introduced.

Even stronger restrictions on lattice parameters (implying $\lambda_2 = 1$) called the *cofactor conditions* are presented in the talk [5]. A material satisfying the cofactor conditions has not yet been discovered. Also presented is a startling new alloy [6] in the Heusler family that was discovered by the kind of tuning of $\lambda_2$ described above. It has nonferromagnetic martensite but strongly ferromagnetic austenite. It raises a host of profound theoretical questions.

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[2]The question of an appropriate definition of local minimizer is intertwined with the question of what is the appropriate model of interfacial energy for these materials.

[3]The ansatz used in the elementary treatment can be interpreted as a nucleus of the incipient phase being stabilized by a defect.

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# A kinetic theory of shock clustering in scalar conservation laws
## Govind Menon

We describe a kinetic theory for shock clustering in scalar conservation laws with random initial data. Our main discovery is that for a natural class of random data the shock clustering is described by a completely integrable Hamiltonian system. Thus, the problem is in a precise sense *exactly solvable*. Our results have implications in other areas: mathematical physics (limits of shell models of turbulence, and forced Burgers turbulence); probability theory (explicit computations of laws of excursions); and statistics (limit laws in the vicinity of maxima).

Our work grew out of a study of Smoluchowski's coagulation equation. This is a mean-field model of domain coarsening, first introduced to model coagulation in colloids. Quite remarkably, it also describes the clustering of shocks in Burgers equation for a class of random initial data [3, 7, 12]. This is a particular case of *Burgers turbulence*– the study of shock statistics in Burgers equation with random initial data or forcing. Our goal was to understand if this link between a mean-field model of coalescence and shock clustering was an isolated example, or part of a more general theory. It is in fact, a consequence of the theory outlined below.

*The problem.* We consider the scalar conservation law

$$(1) \qquad \partial_t u + \partial_x f(u) = 0, \quad x \in \mathbb{R}, \ t > 0,$$

with a $C^1$ convex flux function $f$ and random initial data $u(x,0) = u_0(x)$. The entropy solution to (1) is given by the Hopf-Lax formula. Thus, (1) induces the evolution of the law of $u_0$. The problem is to determine this evolution.

The main assumption we make is that $u_0$ is a Markov process (in $x$) with only downward jumps. This assumption is motivated by some remarkable exact solutions in Burgers turbulence. Burgers considered white noise initial data in his pioneering work on statistical hydrodynamics [4, 5, 6]. The same problem also arose in statistics [9], and was solved in this context by Groeneboom [10]. He showed that for every $t > 0$, the process $u(x,t)$, $x \in \mathbb{R}$ is a stationary Markov process with only downward jumps, and he computed the generator of this process explicitly. There are two remarkable aspects to his solution: the first is the 'structural' fact that the Hopf-Lax formula respects the Markov property of $u_0$. The second is that the law of $u(x,t)$ can be computed *explicitly*. We now explain how both features hold in generality.

*Kinetic theory and Lax equations.* This part is joint work with Ravi Srinivasan [13]. The following *closure theorem* holds: if $u(x, 0)$ is a Markov processes with only downward jumps, then so is the entropy solution $u(x, t)$, $t > 0$.

Markov processes with some regularity (Feller processes) are characterized by their generators. For example, if $u(x, t)$ is a stationary, spectrally negative Feller process in $x$, its generator $\mathcal{A}(t)$ acts on test functions $\varphi \in C_c^1(\mathbb{R})$ via

$$(2) \qquad \mathcal{A}\varphi(y) = b(y, t)\varphi'(y) + \int_{-\infty}^{y} (\varphi(z) - \varphi(y)) \, n(y, dz, t).$$

These terms correspond to the drift and jumps (i.e. rarefactions and shocks) of $u$.

The closure theorem reduces the problem of evolution of shock statistics to a study of the evolution of the generators. One of our main results is that the evolution of $\mathcal{A}$ is given by the Lax equation

$$(3) \qquad \partial_t \mathcal{A} = [\mathcal{A}, \mathcal{B}] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A}.$$

Here $\mathcal{B}$ is defined by its action on test functions as follows:

$$(4) \qquad \mathcal{B}\varphi(y) = -f'(y)b(y, t)\varphi'(y) - \int_{-\infty}^{y} \frac{f(y) - f(z)}{y - z} (\varphi(z) - \varphi(y)) \, n(y, dz, t).$$

It requires considerable insight to realize that this approach is fruitful, and our work was greatly inspired by Duchon and his co-workers [7, 8]. In particular, (3) simplifies and generalizes their work. The Lax equation (3) expands (using (2)) to yield kinetic equations of shock clustering for $b$ and $n$. All known exact solutions to Burgers turbulence satisfy (3).

*Hamiltonian structure and geodesic flows of Markov operators.* Lax pairs are synonymous with completely integrable systems. We also noted other 'integrable properties' in [13] (a Painlevé property, connections with random matrices, and more). Much of our work since the discovery of (3) has been devoted to understanding this structure. The following picture has emerged, though many aspects remain to be pinned down.

To show that (3) is a Hamiltonian system we must introduce a phase space, a symplectic structure and a Hamiltonian. This is done by discretization and a passage to the limit. We restrict $u(x, t)$ to a Markov process on an $n$-dimensional state space. In this case $\mathcal{A}$ is an $n \times n$ matrix (say $A$), and (3) yields a matrix evolution equation $\dot{A} = [A, B]$ where $B_{ij} = F_{ij}A_{ij}$ is a natural discretization of (4). This is a Hamiltonian system with the symplectic structure of Kostant and Kirillov and a quadratic Hamiltonian $H(A) = \sum_{ij} A_{ij}B_{ij}$. In the limit $n \to \infty$, we find that (3) is a Hamiltonian flow on a Lie algebra of generators of Markov processes. When $f' > 0$, (3) formally describes geodesic flows on a space of Markov processes with metric determined by $f$.

*The spectral curve and algebraic complete integrability.* The fact that (3) is *completely integrable* appears to follow from the following simple observation. Let $\mathcal{M}$ and $\mathcal{N}$ denote multiplication operators acting on the domain of $\mathcal{A}$, defined by

$$(5) \qquad \mathcal{M}\varphi(y) = y\varphi(y), \quad \mathcal{N}\varphi(y) = f(y)\varphi(y).$$

It is clear that $\mathcal{M}$ and $\mathcal{N}$ are diagonal operators. We now use the definitions (2), (4) and (5) to find

$$(6) \qquad\qquad [\mathcal{A}, \mathcal{N}] - [\mathcal{M}, \mathcal{B}] = 0.$$

This observation allows us to introduce a spectral parameter $\mu \in \mathbb{C}$ in the Lax equation. We use (3) and (6) to obtain

$$(7) \qquad\qquad \partial_t (\mathcal{A} - \mu\mathcal{M}) = [\mathcal{A} - \mu\mathcal{M}, \mathcal{B} + \mu\mathcal{N}], \quad \mu \in \mathbb{C}.$$

If $\mathcal{A}$, $\mathcal{B}$ were $n \times n$ matrices, it would follow that the spectral curve (Riemann surface)

$$(8) \qquad\qquad \Gamma = \{(\lambda, \mu) \in \mathbb{C}^2 \,|\, \det(\mathcal{A} - \lambda\,\mathrm{id} - \mu\mathcal{M}) = 0\},$$

is fixed by the evolution. This is the crucial observation that yields the existence of additional integrals for Euler's equations in $so(n)$, $n \geq 4$ in Manakov's treatment of Euler's equations [11]. These integrals are simply the coefficients of the characteristic polynomial above.

This observation shows that the discretizations of (3) describe completely integrable flows on the 'Markov' group $\{A \in gl(n) | \sum_{j=1}^n A_{ij} = 1, i = 1, \ldots, n\}$ in precise analogy with Manakov's work. More broadly, it reveals a close relation with a large class of completely integrable systems (including KdV, the Toda lattice, geodesic flows on $so(n)$ and ellipsoids, and the integrable PDEs of random matrix theory). The complete integrability of all these flows may be obtained in a unified way via a general splitting theorem for Lie algebras [1]. This connection also sets the stage for the application of powerful methods from algebraic geometry to integrate (3) explicitly for *every* convex $f$ [2].

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# Droplet phases in non-local Ginzburg-Landau models with Coulomb repulsion in two dimensions

## Cyrill B. Muratov

Spatial patterns are often a result of the competition between thermodynamic forces operating on different length scales. When short-range attractive interactions are present in a system, phase separation phenomena can be observed, resulting in aggregation of particles or formation of droplets of new phase, which evolve into macroscopically large domains via coarsening or nucleation and growth [1]. This process, however, can be frustrated in the presence of long-range repulsive forces. As the droplets grow, the contribution of the long-range interaction may overcome the short-range forces, whereby suppressing further growth.

One important class of systems with competing interactions are systems in which the long-range repulsive forces are of Coulomb type (for an overview, see [2, 3] and references therein). The nature of the Coulombic forces may be very different from system to system. For example, these forces may arise when particles undergoing phase separation carry net electric charge [4, 5, 6, 7], or they may be a consequence of entropic effects associated with chain conformations in polymer systems [8, 9, 10]. Coulomb interactions may also arise indirectly as a result of diffusion-mediated processes [11, 12, 13]. All this makes systems with repulsive Coulombic interactions a ubiquitous example of pattern forming systems.

Motivated by the above discussion, we consider the following energy functional on $\mathcal{A} = \{u \in H^1(\Omega) : \frac{1}{|\Omega|} \int_\Omega u \, dx = \bar{u}\}$:

$$\mathcal{E}[u] = \int_\Omega \left( \frac{\varepsilon^2}{2} |\nabla u|^2 + W(u) + \frac{1}{2}(u - \bar{u})(-\Delta^{-1})(u - \bar{u}) \right) dx,$$

where $\Omega$ is a $d$-dimensional torus for simplicity. Here $W$ is a symmetric double-well potential with minima at $\{-1, 1\}$, and the parameter $\varepsilon > 0$ is the dimensionless surface tension. We are particularly interested in the case $\varepsilon \ll 1$, which gives rise to interfacial patterns. From the basic balance of interfacial and long-range forces it is clear that these interfacial patterns should have length scale $R \sim \varepsilon^{1/3}$ [8, 2, 3, 14]. In fact, if the size of the domain $\Omega$ is also assumed to have the same scaling, then it is possible to formulate a reduced energy functional in terms of only the interfacial positions, using the methods of $\Gamma$-convergence [15, 16, 17, 18, 19]. At the same time, when the size of $\Omega$ is $O(1)$, i.e. it is of order or exceeding the Debye screening length in the considered system, then in the limit $\varepsilon \to 0$ the energy minimizing patterns exhibit small-scale oscillations, presenting difficulties for this approach.

Our first result concerning the behavior of energy minimizers for energy $\mathcal{E}$ provides a rigorous justification for the reduced sharp interface energy $E$ obtained formally in [2, 3], whose minimum value has the same asymptotic behavior as $\varepsilon \to 0$ [20]. We show that when the space dimension $d$ is not too high (in particular, in the physically relevant dimensions $d \leq 3$), it is appropriate to consider the following energy functional

$$E[u] = \int_\Omega \left( \frac{\varepsilon}{2} |\nabla u| + \frac{1}{2} (u - \bar{u})(-\Delta + \kappa^2)^{-1}(u - \bar{u}) \right) dx,$$

defined for all $u \in BV(\Omega; \{-1, 1\})$, where $\kappa = 1/\sqrt{W''(1)}$ is the screening parameter. We then concentrate on the specific case $d = 2$ and show that near the transition from trivial to non-trivial minimizers of $E$ occurring at $1 + \bar{u} = O(\varepsilon^{2/3} |\ln \varepsilon|^{1/3})$, the energy minimizers (i.e., sets where $u = +1$) consist of $O(|\ln \varepsilon|)$ nearly perfect disks of size $r \simeq (3\varepsilon/|\ln \varepsilon|)^{1/3}$ uniformly distributed across $\Omega$.

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# Self-similar solutions for coagulation equations

BARBARA NIETHAMMER

(joint work with J.J.L. Velázquez)

We consider Smoluchowski's classical coagulation equations that describe the evolution of the number density $f(t, x)$ of clusters of mass $x$. Clusters of size $x$ and $y$ can coalesce by binary collisions to clusters of size $x + y$ at a rate given by a rate kernel $K(x, y)$. Thus the dynamics of $f$ are given by

$$
(1) \quad \begin{aligned}
\frac{\partial}{\partial t} f(t, x) &= \frac{1}{2} \int_0^x K(y, x - y) f(t, x - y) f(t, y) \, dy \\
&\quad - f(t, x) \int_0^\infty K(x, y) f(t, y) \, dy,
\end{aligned}
$$

supplemented with initial conditions at $t = 0$. The qualitative behaviour of solutions to (1) depends crucially on the form of the rate kernel $K(x, y)$ in which all the physics of the underlying process are subsumed. Depending on the properties of $K$, the total mass of clusters is preserved for all times or clusters of infinite size are created in finite time, a phenomenon known as gelation.

We are here interested in the first case where mass is transported to larger and larger clusters, but the total mass is preserved for all times. For simplicity we restrict ourselves here to the two examples of rate kernels

$$
(2) \quad K_1(x, y) = x^\gamma + y^\gamma \quad \text{and} \quad K_2(x, y) = x^{\gamma/2} y^{\gamma/2}, \quad \gamma \in [0, 1),
$$

that are called the sum- and multiplicative kernel respectively.

In this talk we describe some results and open problems in the topic of dynamic scaling that concerns the existence of self-similar solutions and their domains of attraction. For the class of kernels described above this issue is only well-understood for the constant kernel. In this case there exists an explicit exponentially decaying self-similar solution and recently a new family of self-similar solutions with algebraic decay has been discovered and their domains of attraction have been characterized [6]. However, the proofs rely on the use of the Laplace transform and thus the methods cannot be applied to the kernels in (2) if $\gamma \in (0, 1)$. For such kernels dynamic scaling is much less understood. The existence of mass-conserving self-similar solutions for a class of homogeneous kernels that include $K_1$ and $K_2$ has been established in [2, 4]. Further estimates on their precise decay at infinity and their behaviour for small clusters have been derived in [4, 5, 1, 3]. For the sum kernel $K_1$ these results are optimal in the sense that they agree with the behavior predicted by formal asymptotic analysis, for the multiplicative kernel, however, they are only supoptimal.

In this talk we present some results on mass-conserving self-similar solutions for the multiplicative kernel. More precisely we prove that a self-similar solutions $\phi(x)$ behaves as $\phi(x) \sim x^{-(1+\gamma)}$ as $x \to 0$. This improves the so far best results for the multiplicative kernels that was obtained in [3]. It is furthermore expected that $\lim_{x \to 0} x^{1+\gamma} \phi(x) = c_0(\gamma)$ with a specific constant $c_0(\gamma)$ but we are presently not able to prove this. Furthermore, a formal analysis of the next order asymptotics show that solutions behave oscillatory and thus it is not surprising that the continuity result is difficult to obtain. We outline a strategy for constructing self-similar solutions with the expected behavior for small $\gamma$ that relies on a shooting type argument.

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# Stability of planar fronts for a non–local phase kinetics equation with a conservation law in $D \leq 3$

Enza Orlandi

(joint work with E. A. Carlen)

We consider, in a $D-$dimensional cylinder, a non–local equation that describes the evolution of the local magnetization in a continuum limit of an Ising spin system with Kawasaki dynamics and Kac potentials. We consider sub–critical temperatures, for which there are two local homogeneous in space equilibria, and show a local nonlinear stability result for the planar fronts connecting these two different local equilibria. Further, we shall show that an initial perturbation of a front that is sufficiently small in $L^2$ norm, and sufficiently localized yields a solution that relaxes to another front, selected by a conservation law, in the $L^1$ norm at an algebraic rate that we explicitly estimate. We also obtain rates for the relaxation in the $L^2$ norm and the rate of decreasing of the excess free energy.

We analyze the following nonlocal and nonlinear evolution equation:

(1)
$$\frac{\partial}{\partial t}m(x,t) = \nabla \cdot \left(\nabla m(x,t) - \beta(1 - m(x,t)^2)(J \star \nabla m)(x,t)\right) \quad x \in R \times \Lambda,$$
$$m(0,x) = m_0(x), \quad m_0(x) \in [-1,1]$$

where $\Lambda$ is a $(D-1)-$ dimensional torus of edge $L > 1$, $\beta > 1$, $\star$ denotes convolution, $J$ is smooth, spherically symmetric probability density with compact support. This equation first appeared in the literature in a paper [7] on the dynamics of Ising systems with a long–range interaction and so–called "Kawasaki" or "exchange" dynamics. In this physical context, $m(x,t)$ is the magnetization density at $x$ at time $t$, viewed on the length scale of the interaction, and $\beta$ is the inverse temperature. The derivation of (1) from the underlying stochastic dynamics with $x$ taking values in a torus $T^d$ is done in [5]. Equation (1) has been object of several studies.

Basic to our work is that the equation (1) can be written in a gradient flow form. To do this, we introduce the free energy functional $\mathcal{F}(m)$ where

(2)
$$\mathcal{F}(m) = \int_{R \times \Lambda} [f(m(x)) - f(m_\beta)]dx + \frac{1}{4}\int_{R \times \Lambda}\int_{R \times \Lambda} J(x-y)[m(x) - m(y)]^2 dxdy$$

and $f(m)$ is

(3)
$$f(m) = -\frac{1}{2}m^2 + \frac{1}{\beta}\left[\left(1 + \frac{m}{2}\right)\ln\left(1 + \frac{m}{2}\right) + \left(1 - \frac{m}{2}\right)\ln\left(1 - \frac{m}{2}\right)\right].$$

For $\beta > 1$, this potential function $f$ is a symmetric double well potential on $[-1,1]$. We denote the positive minimizer of $f$ on $[-1,1]$ by $m_\beta$. It is easy to see that $m_\beta$ is the positive solution of the equation

$$m_\beta = \tanh(\beta m_\beta).$$

The functional (2) is well defined although it might be infinity. The equation (1) can be written as

(4)
$$\frac{\partial}{\partial t}m = \nabla \cdot \left(\sigma(m)\nabla\left(\frac{\delta \mathcal{F}}{\delta m}\right)\right)$$

where the *mobility* $\sigma(m)$ is given by

(5)
$$\sigma(m) = \beta(1 - m^2),$$

and the formal Frechet derivative of the free energy $\frac{\delta \mathcal{F}}{\delta m}$ is

(6)
$$\frac{\delta \mathcal{F}}{\delta m} = \frac{1}{\beta}\text{arctanh}(m) - J \star m.$$

Then, formally one derives

(7)
$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(m(t)) = -\int_{\mathbb{R} \times \Lambda}\left|\nabla\left(\frac{\delta \mathcal{F}}{\delta m}\right)\right|^2 \sigma(m(t))dx = -\mathcal{I}(m(t))$$

thus $\mathcal{F}$ is a Lyapunov function for (1). This suggests that the free energy should want to tend locally to one of the two minimizing values, $\pm m_\beta$, and that the interface between a region of $+m_\beta$ magnetization and a region of $-m_\beta$ 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. Consider a planar interface with $m$ positive for $x_1 \geq 0$ and $m$ negative for $x_1 \leq 0$. In [4] is was shown that there exists an unique function $\bar{m}_0(x_1)$ such that

$$\mathcal{F}_1(\bar{m}_0) = \inf \left\{ \mathcal{F}_1(m) \,\middle|\, \mathrm{sgn}(x_1)m(x_1) \geq 0, \lim_{x_1 \to \pm\infty} \mathrm{sgn}(x_1)m(x_1) > 0 \right\},$$

where $\mathcal{F}_1$ is is the functional (2) in $d = 1$ with interaction $\bar{J}(x_1) = \int_\Lambda J(x_1, x^\perp)\mathrm{d}x^\perp$. A review of these and related results can be found in Chapter 8 of the book [8]. For any $a$ in $\mathbb{R}$, define

$$\bar{m}_a(x) = \bar{m}_a(x_1, x_1^\perp) = \bar{m}_a(x_1) = \bar{m}_0(x_1 - a), x \in \mathbb{R} \times \Lambda$$

where we denoted by $x_1^\perp \in \Lambda$. These functions $\bar{m}_a$ are stationary solutions of (1) whose stability is to be investigated here. Clearly

$$\mathcal{F}(\bar{m}_a) = \mathcal{F}(\bar{m}_0), \qquad \frac{\delta\mathcal{F}}{\delta m}(\bar{m}_a) = \frac{1}{\beta}\mathrm{arctanh}(\bar{m}_a) - J \star \bar{m}_a = 0.$$

The equation (1) not only has a Lyapunov function; it has a conservation law as well: For times $t$ in any interval on which $m(t) - \mathrm{sgn}(x_1)m_\beta$ is integrable,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R} \times \Lambda} \big(m(x, t) - \bar{m}_b(x)\big)\mathrm{d}x = 0$$

for any $b$. Therefore, if one defines $a$ in terms of the initial data $m_0$ for (1) by

$$(8) \qquad \int_{\mathbb{R} \times \Lambda} \big(m(x, 0) - \bar{m}_a(x)\big)\mathrm{d}x = 0,$$

one has for the solution

$$\int_{\mathbb{R} \times \Lambda} \big(m(x, t) - \bar{m}_a(x)\big)\mathrm{d}x = 0$$

for all $t$ or at least all $t$ such that $m(s, x) - \mathrm{sgn}(x_1)m_\beta$ is integrable for all $s \leq t$. Now formally invoking the Lyapunov function and the conservation law, it is easy to guess the result of solving (1) for initial data $m_0$ that is a small perturbation of the front $\bar{m}_0$: The decrease of the excess free energy should force the solution $m(t)$ to tend to the family of fronts, and the conservation law should select $\bar{m}_a$ as the front it should be converging to, so the result should be that

$$\lim_{t \to \infty} \int_{\mathbb{R} \times \Lambda} |m(x, t) - \bar{m}_a(x)|\mathrm{d}x = 0,$$

with $a$ given in terms of the initial data $m_0$ through (8). The main result obtained is the following.

**Theorem 0.1.** *Let $m(t)$ be the solution of equation* (1) *in the $D-$ dimensional cylinder, $D \leq 3$, and with initial data $m_0(x)$ such that*

$$\int_{\mathbb{R} \times \Lambda} x_1^2 (m_0(x) - \bar{m}_0(x))^2 \mathrm{d}x \leq c_0 \ ,$$

*where $c_0$ is any positive constant. Then for any $\delta > 0$ there is a strictly positive constant $\epsilon = \epsilon(\delta, c_0, \beta, J, L)$ such that for all initial data $m_0$ with $-1 \leq m_0 \leq 1$, and with*

$$\int_{\mathbb{R} \times \Lambda} (m_0(x) - \bar{m}_0(x))^2 \mathrm{d}x \leq \epsilon \ ,$$

*the excess free energy $\mathcal{F}(m(t)) - \mathcal{F}(m_0)$ of the corresponding solution $m(t)$ of* (1) *satisfies*

$$\mathcal{F}(m(t)) - \mathcal{F}(\bar{m}) \leq c_2 (1 + c_1 t)^{-(9/13 - \delta)}$$

*and*

$$\int_{\mathbb{R} \times \Lambda} |m(t, x) - \bar{m}_a(x)| \mathrm{d}x \leq c_2 (1 + c_1 t)^{-(5/52 - \delta)}$$

*where $c_1$ and $c_2$ are finite constants depending only on $\delta$, $c_0$, $J$, $\beta$ and $L$ and $a$ is given by* (8).

In $D = 1$ the same stability problem for the equation (1) was addressed in the papers [1] and [2]. The strategy used in these papers was applied in [3], always in $D = 1$ to a similar problem for Cahn-Hilliard equation.

The method applied in $D = 1$ has been adapted in this paper to show local non linear stability of the planar fronts of (1) when dimension $D > 1$. To apply the previous strategy in $D > 1$ one needs to control the transvers contribution of the perturbation to the planar fronts. This is done by a clever splitting of a function in $R \times \Lambda$ as the sum of two functions, one depending only on $x_1 \in R$ and the other with mean zero in the direction orthogonal to $x_1$. This allows to suitable split the problem and to control the gradient of the function in the transvers direction applying the Poincaré inequality. The method is robust enough and it should allow to deal with nonlinear local stability problems for other equations as Cahn-Hilliard type in $D \leq 3$. Nonlinear local stability results for the planar fronts for Cahn- Hilliard equation were obtained in $D \geq 3$ by [6].

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## Scaling limits in some mean-field domain-growth models

ROBERT L. PEGO

(joint work with G. Menon, B. Niethammer, J. Carr)

We discuss long-time dynamic behavior in several rate-equation models of domain growth that involve coagulation, or aggregation of domains. Two of the models are motivated by the dynamics of domain walls in the 1-D Allen-Cahn equation. When the potential-well depths are equal, the rate equation models a simple domain-collapse dynamics: The smallest domain collapses instantaneously, joining with its two neighbors to form one larger domain. Simulations show convergence to a self-similar form that corresponds to a self-similar size distribution whose Laplace transform is $\tanh(\frac{1}{2}\mathrm{Ei}(q))$ [1]. A remarkable solution procedure for this model was found by Gallay and Mielke [2], and used to establish a number of strong results involving rates of convergence to self-similar form.

With G. Menon and B. Niethammer [3], we have recently (i) extended well-posedness theory to handle size distributions that are arbitrary measures with support bounded away from 0; (ii) established necessary and sufficient conditions on initial data for solutions to have a single proper scaling limit as $t \to \infty$; and (iii) provided a Lévy-Khintchine representation formula for so-called *eternal solutions*, which exist for all possible times in this model. The criterion for a scaling limit is that the first-moment distribution function is regularly varying (i.e., power law up to a factor that is slowly varying at infinity). The proofs involve simple scaling rigidity arguments as one finds in Feller's book, combined with the delicate exponential Tauberian theorem of de Haan. One curious point involves multiple collisions: $k$ clusters can coalesce with probability $p_k$. When $\Sigma p_k k \log k = \infty$, the scaling symmetry of the model is broken, up to a slowly varying factor, which can nevertheless be dealt with.

In ongoing work with Jack Carr (Heriot-Watt), we study domain walls that move at a constant speed, leading alternately to uniformly shrinking and growing domains. When a shrinking domain reaches zero size, its two growing neighbors join. The size distribution of shrinking domains has trivial dynamics, but its initial value provides the time history of the coagulation rate for growing domains. We can classify initial data that lead to self-similar growth in the case that initially the distribution of growing domains has a heavier tail that that of shrinking domains. When the initial tail for shrinking domains dominates, the limiting profile can have

a distribution that agrees with that for the ratio of a sum of IID random variables to the largest term in the case when the underlying distribution is $\alpha$-stable.

Finally, for Smoluchowski's coagulation equation with the solvable kernel $K = x + y$, we discuss results obtained with Govind Menon [4] regarding the *scaling attractor*, which is the set of cluster points of rescaled mass distributions $F_t(dx)$ for solutions:

**Definition.** A probability measure $\hat{F}(dx)$ on $[0, \infty]$ is a point in the scaling attractor $A$ if there exist a sequence of positive numbers $b_n \to \infty$ and a sequence of solutions all defined for $t \in (0, \infty)$ such that the corresponding mass distribution functions satisfy

$$F_{t_n}^{(n)}(b_n dx) \to \hat{F}(dx) \quad \text{weakly as } n \to \infty.$$

Points in the scaling attractor are the values at $t = 0$ of eternal solutions defined for all $t \in (-\infty, \infty)$ (possibly extended to include 'dust' and 'gel' that concentrate probability at 0 and $\infty$). In turn, due to a result of Bertoin, eternal solutions are parametrized in terms of a family of "g-measures" $G$. This family is defined by the property that $(1 \wedge x^{-1})G(dx)$ is a finite measure on on $[0, \infty]$. These measures are rather well-known in probability theory as the Lévy measures corresponding to (killed) subordinators. The rescaled measures $G_t(dx) = xe^{-t}F_t(e^t dx)$ g-converge to a limiting g-measure $G_*(dx)$. And every g-measure corresponds to a unique enternal solution in this way.

This induces a bicontinuous bijection between the scaling attractor and the family of g-measures. Remarkably, the nonlinear dynamics on the scaling attractor becomes purely dilational in terms of the representing g-measure: the time-$t$ map $\hat{F}_0 \mapsto \hat{F}_t$ on the scaling attractor corresponds to the map

$$G_*(dx) \mapsto e^{2t}G_*(e^{-t}dx)$$

on g-measures. By consequence, the time dynamics is conjugate to continous-time shift dynamics, and we can exhibit a number of signatures of chaotic dynamics (sensitivity to the initial tails of the size distribution): a dense set of scaling-periodic solutions; a single solution trajectory with scaling limits dense in the scaling attractor; and an asymptotic shadowing result for solutions with similar initial tails. Many of these results and their proofs are strongly analogous to classical limit theorems concerning infinitely divisibility in probability theory.

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# Nanoscale precursor textures of martensitic phase transitions

Antoni Planes

(joint work with T. Castán, P. Lloveras, M. Porta, A. Saxena)

Spatially inhomogeneous states often occur as precursors to a phase transition in many ferroic materials such as ferroelastic, ferroelectric, magnetic and superconducting among others [1, 2]. These textures usually consist of a multi-phase pattern of coexisting regions with properties varying over nanometer distances [3, 4]. Usually, even when the strain is not a primary order parameter, it plays a crucial role in determining the actual symmetry properties of nanoscale patterns. From this point of view martensites (and in general ferroelastic materials) offer a unique scenario where purely structural textures can be studied.

Martensites are crystal structures that originate through a displacive solid-solid transformation. Commonly they take place from an open cubic phase to a nearly close-packed structure with significant first-order character [5]. In the simplest cases of non-modulated martensites, the order parameter consists of the relevant components of the strain tensor describing the unit cell distortion. This distortion is related to the existence of specific soft directions (usually related to the elastic constant $C'$) that render the material elastically anisotropic [6]. In these systems, cross-hatched strain modulations (the so-called tweed patterns) often appear well above the actual transition temperature. These precursors can be detected as contrast anomalies in TEM and consist of diffuse striations parallel to the traces of specific planes of the high symmetry phase [7, 8]. No signature of tweed contrast has however been observed in some martensitic materials such as those of the Ti-Ni alloy family. Instead, in these alloys nanodomains of the incoming phase of almost spherical shape occur as precursors to the martensitic phase [9, 10]. Moreover, under some circumstances, the transition to the martensitic phase is inhibited and instead the system shows glassy behavior characterized by the splitting of strain vs. temperature curves after cooling with or without stress which reveals history dependent effects [11]. It has been suggested [9] that this peculiar behaviour might be related to a low value of elastic anisotropy. In Ti-Ni alloys this low anisotropy results from an anomalously small value of the elastic shear constant $C_{44}$.

The essential ingredients that enable a martensitic transition to be preceded by tweed are: (i) the system must show high sensitivity (in the sense of response functions) to local symmetry breaking perturbations arising from disorder in the form of lattice defects, point defects, inhomogeneities, etc. resulting in long-lived fluctuations of the low-symmetry phase. (ii) Long range interactions are needed to produce a global response and (iii) anisotropy is crucial in order to select specific directions for modulations. The aim now is to propose a model where the role of the above factors can be analysed separately.

For the sake of simplicity we consider a 2-$d$ square-rectangular transition. Let $e_1$, $e_2$, and $e_3$ denote symmetry adapted strains, respectively, for hydrostatic, deviatoric and shear distortions of the square lattice. The change of symmetry at

the transition is described by $e_2$ that will be the (primary) order parameter. Soft-directions will be along $\{11\}\langle1\bar{1}\rangle$ displacements associated with a small elastic constant $C'$. The elastic anisotropy is then measured by the ratio $A = C_{44}/C'$. A general Landau free energy density for this transition will include a non-linear local term in the order parameter adequate for a first-order transition together with the elastic energy associated with non-symmetry breaking strains and a gradient term accounting for the energy cost of interfaces. This free energy must be minimized imposing elastic compatibility through the Saint-Vénant condition for the geometrically linear strain tensor $\varepsilon$ , $\vec{\nabla} \times (\vec{\nabla} \times \varepsilon)^T = 0$ (see for instance ref. [8]), which mathematically expresses the requirement of lattice integrity without creating any topological defects. The following effective free energy density is then found:

$$(1) \quad f(e_2, T) = \frac{1}{2}C'(T)e_2^4 - Be_2^2 + De_2^6 + K(\vec{\nabla}e_2)^2 + \int d\vec{r'}\, e_2(\vec{r})U(|\vec{r} - \vec{r'}|)e_2(\vec{r'}).$$

In $k$-space the kernel of the non-local term is given by

$$(2) \qquad\qquad U(k_x, k_y) = \frac{C_{44}}{2}\frac{\left(k_x^2 - k_y^2\right)^2}{Rk^4 + 8(k_x k_y)^2},$$

where $R = C_{44}/(C_{11} + C_{12})$ is the ratio between the shear and the bulk moduli. The strength of this long range term depends on $C_{44}$ and therefore increases with the elastic anisotropy. This term is minimized for $k_x = \pm k_y$ which explains the directionality of long range correlations along the diagonals.

Disorder is introduced in the model taking into account that: (i) in any alloy, composition is not strictly homogeneous, but instead, composition fluctuations are known to occur, and (ii) in martensitic systems, the transition temperature is strongly dependent on composition. Consequently, we assume that disorder arises from composition fluctuations that give rise to a certain distribution of local transition temperatures. Formally, the harmonic coefficient $C'$ in (1) is assumed to be of the form: $C' = a[T - T_c - \eta(\vec{r})]$, where $\eta$ denotes a spatially fluctuating field and $T_c$ the low stability limit of the high temperature phase in the clean limit (i.e., in the absence of disorder). The field is taken to be spatially correlated and gaussian distributed with zero mean in order to mimic smooth variations of composition in space. This gives rise to a spatial distribution of transition temperatures, $T_t(\vec{r}) = T_0 + \eta(\vec{r})$ (where $T_0 = T_c + 3B^2/16aD$ is the equilibrium transition temperature of the model in the clean limit). The standard deviation $\zeta$ of this distribution conveniently quantifies the amount of disorder. Therefore, regions with different degree of metastability separated by finite free energy barriers exist in the system.

Numerical simulations (using a pure relaxational dynamics) show that in the limit of high anisotropy and/or low disorder, when the system is cooled down (cross-hatched) tweed textures appear at high temperature and on further cooling the phase transition to a long range ordered twinned martensitic phase takes place. In contrast, for low values of the elastic anisotropy and/or high disorder, instead of tweed droplets of the low temperature phase occur at high temperature. In this

case, the transition to the martensitic phase is suppressed and instead a ramified droplet-like structure (phase-separated state) continuously grows as temperature is decreased. Moreover, in this phase separated state the system exhibits glassy behaviour at low-enough temperatures which can be characterized from the splitting of strain vs. temperature curves obtained upon heating, following a cooling under zero stress (ZFC) in one case, and under non-zero stress (FC) in the other. Indeed, this is a proof of history dependence. It is worth pointing out that the observed glassy behaviour is of kinetic origin due to the existence of the local energy barriers arising from disorder and that no geometrical frustration plays a role associated with such glassy states [12]. These results are in very good agreement with experiments reported in Ti-Ni-based alloys [11, 13, 14].

Another interesting aspect to be studied is the effect of an external stress in the phase separated state. The coupling with the external stress, $\sigma$, is introduced by including a term $(-\sigma e_2)$ in the free energy (1). Simulation results show that regardless of the amount of disorder and value of the elastic anisotropy factor, application of stress induces a single variant martensite. Depending on temperature superelastic or pseudoelastic behaviour is found. In the latter case, upon unloading, the strain is not recovered and instead the single variant state remains stable. When heating up the reverse transition occurs and and the initial undeformed shape is recovered. Therefore, even if the martensitic transition is inhibited, shape-memory effect still occurs. This is also in good agreement with experiments [15].

To conclude, we have shown that properties of precursor textures in ferroelastic/martensitic systems are controlled by the competition between disorder and elastic anisotropy that determines the strength of long range interactions. The presence of disorder gives rise to a distribution of energy barriers that, above a certain critical amount (that does depend on the elastic anisotropy), is able to screen the long-range potential, breaking correlations, and thus suppressing the transition to the martensitic twinned structure. In this case, in agreement with experiments, the system displays glassy behaviour.

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## Rigorous results for the 6-vertex model with domain-wall boundary conditions

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(joint work with Pavel Bleher)

We consider the six-vertex model with domain wall boundary conditions in its antiferroelectric regime. That means that the parameters $a, b, c$ of the model satisfy $\Delta \equiv \frac{a^2+b^2-c^2}{2ab} < -1$. We study the spatial curves separating the disordered zones from the frozen and from the rigid (gaseous) zones. We show that in the limit when $\Delta \to -\infty$ the two lines converge to the boundary of the limiting rectangle.

## Coarsening in Energy-Driven Systems

DEJAN SLEPČEV

(joint work with Eva Eggeling, Matt Elsey, Karl Glasner, Felix Otto, Tobias Rump, Shlomo Ta'asan)

Many energy-driven systems exhibit coarsening behavior. Typically, starting from a high-energy state a system quickly equilibrates locally, while remaining globally far from the equilibrium. The pattern, that initially forms, slowly coarsens over time — the characteristic length scales of its features grow, while the morphology of the patterns changes little. For example initially uniform thin films of di-block copolymers can break up into configuration of droplets. The droplets are connected by an ultra-thin film, through which they interchange mass. In a process similar to Ostwald ripening the large droplets grow at the expense of smaller ones. The number of droplets is decreasing, while their typical size increases.

Coarsening also arises when a binary mixture is quenched to sufficiently low temperature at which the mixture is thermodynamically unstable. The fluids separate, at first locally. A fine labyrinthine pattern forms. Over time this pattern coarsens.

Finally when a melted material (that at low temperatures forms crystal structure) is suddenly cooled below the solidification temperature, it quickly solidifies locally by forming little crystals. However the crystaline orientation of the little crystal grains differs and thus the boundaries between them form. The energy which concentrated at these boundaries then drives the interfacial motion. The grain boundaries move by their mean curvature. This leads to coarsening of the

grain boundary network. The number of grains decreases, while their typical size grows.

The following questions arise in all of the above systems:

(1) What is the rate at which the coarsening progresses? Can it be established rigorously?
(2) What are the features of the patterns that form?
(3) Is the statistics of the patterns selfsimilar it time?

We address a part of the first question. Namely, the question of establishing the rate of coarsening can be split into proving matching upper and lower bounds on the rate. However, in many systems, only the upper bound is universal. More precisely, while one can show that no initial configuration can coarsen faster than a given rate, there are often many configurations that do not coarsen at all. Typically these are unstable steady states or are in other ways dynamically inaccessible from typical initial data, and are thus not seen in experiments. We concentrate on providing upper bounds. A breakthrough on rigorously proving upper bounds on coarsening was made by Kohn and Otto [3] who introduced the technique for obtaining the bounds by proving appropriate estimates on the flatness of the energy landscape, over large distances. Indeed this technique provides optimal (in terms of scaling) upper bounds on the rate of coarsening in the thin-film equation with linear mobility [4].

However when mobility is a power law (with power larger than one), the estimates obtained via the Kohn-Otto approach are no longer optimal. The reason for that is that the Kohn-Otto approach relies on the assumption that the steepness of the energy along a solution path is comparable to the steepness of the energy landscape. In other words, that the solution path between two states is comparable in length to the geodesic connecting the states. For the thin-film equation, the assumption holds when mobility is linear. However when mobility is superlinear the geometry degenerates and there are arbitrarily short paths connecting any two states (of equal mass). Similarly in systems of grain-boundary networks there are arbitrarily short paths connecting any two configurations.

A closer inspection reveals that many of the "near geodesic" (short) paths go through states with high energy (which are thus dynamically inaccessible by gradient flows starting from moderate energies). A natural question that arises is whether considering the geometry restricted to sub-level sets of the energy is enough to prove optimal upper bounds on the rate of coarsening. For grain boundary networks this is sufficient, provided that one is willing to assume that the energy density remains controlled locally, and not just globally. Alternatively one can consider simplified models of grain boundary evolution, such as grain boundary evolution of Voronoi diagrams, where, due to the nature of allowable configurations, no additional assumptions are needed [1].

On the other hand for the evolution of thin liquid films with superlinear mobility even assuming local bounds on energy density is not sufficient to obtain optimal bounds on the rate of coarsening, since the solution paths remain much longer than the geodesic paths. For this system only some asymptotic results on mass transfer

between droplets and on motion of droplets are known [2]. To obtain rigorous results one would need to obtain estimates on the steepness of the energy along the solution paths themselves. This requires better understanding of the dynamics (and not just the energy landscape), and remains largely an open problem.

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## The mixing time of the Ising model with "+" boundary conditions

FABIO TONINELLI

(joint work with P. Caputo, E. Lubetzky, F. Martinelli, F. Simenhaus, A. Sly)

We consider the mixing time of the single spin-flip Glauber dynamics for the Ising model in dimension $d = 2$ and $d = 3$, at low temperature and zero magnetic field, with "+" boundary conditions. The Hamiltonian of the system in a domain $\Lambda$ of $\mathbb{Z}^d$ is

$$(1) \qquad H_\Lambda(\sigma) = - \sum_{i,j \in \Lambda : |i-j|=1} \sigma_i \sigma_j - \sum_{i \in \Lambda, j \in \partial\Lambda : |i-j|=1} \sigma_i$$

where $\sigma_i, i \in \Lambda$ are spin variables which takes values $\pm 1$. The Gibbs measure is given by

$$(2) \qquad \pi_\Lambda(\sigma) = \frac{e^{-\beta H_\Lambda(\sigma)}}{Z_\Lambda(\beta)}$$

where $\beta$ is the inverse temperature.

The Glauber dynamics is a continuous-time Markov process which can be described as follows: to each $i \in \Lambda$ is associated an independent clock which rings at random times, such that the differences between two successive rings is an exponential random variable of mean 1. When the clock at $i$ rings at time $t$, we update $\sigma_i$ by sampling it from the measure $\pi_\Lambda$, conditioned on the value of the spins $\sigma_j, j \neq i$ at time $t$.

We are interested in the speed of convergence of the process to the invariant and reversible measure $\pi_\Lambda$. Speed of convergence can be measured i.e. via the inverse of the spectral gap of the generator, or via the "mixing time" $T_{mix}$, which measures speed of convergence in variation distance.

We always take $\beta$ to be larger than the inverse of the critical temperature of the model, and for definiteness we let $\Lambda$ be a $d$-dimensional cube of side $L$. A long-standing conjecture [3, 1] is that the mixing time is of order $L^2$ for every

$d \geq 2$. The heuristics behind such belief is based on the fact that an initial bubble of the wrong phase (the minus phase) should shink via motion by mean curvature in a time of order $L^2$. Also, in [1] arguments were given which suggest that the spectral gap behaves like $const/L$ in dimension $d = 2$ and is of order 1 (or possibly $(\log L)^{-c}$ for some $c > 0$) in dimension $d = 3$.

The rigorous results available before our study were the following:

- if $d = 2$ and $\beta \gg \beta_c$, then $T_{mix} \leq \exp(c_\epsilon L^{1/2+\epsilon})$ for every positive $\epsilon$ [7];
- if $d = 2$ and $\beta = \infty$, then $L^2/(\log L)^{1+\delta} \leq T_{mix} \leq cL^2$ for suitable constants $c, \delta$ [4];
- if $d = 2$ and $\beta > \beta_c$, then the spectral gap is smaller than $const/L$;
- if $d = 3$ and $\beta \gg \beta_c$, then $T_{mix} \leq \exp(cL(\log L)^c)$ for a suitable $c$ [9];
- if $d = 3$ and $\beta = \infty$ then $T_{mix} \leq cL^3$ [4].

In [8, 6] we considerably improve the result in dimension $d = 2$, by showing that $T_{mix} \leq \exp(c(\beta)(\log L)^2)$ for every $\beta > \beta_c$. In [2], we consider instead the case of $\beta \geq C \log L$ with $C$ sufficiently large (a particular case is $\beta = \infty$). In this case we can prove:

- for $d = 2$, one has $T_{mix} \geq c'L^2$, which matches the upper bound given in [4];
- for $d = 2$, there exist constants $c, c'$ such that the gap is larger than $c/L$ and smaller than $c'/L$;
- for $d = 3$, one has $T_{mix} \leq cL^2(\log L)^c$ for suitable $c$.

For the three-dimensional results, we heavily employ estimates on the zero-temperature fluctuations of tilted Ising interfaces, which can be obtained through estimates on height fluctuations of dimer coverings of the infinite honeycomb lattice [5]. Our result $T_{mix} \leq cL^2(\log L)^c$ in dimension 3 (and especially the proof technique we use) is a first step towards the microscopic justification of mean curvature motion (or suitable modification thereof, which keeps into account the non-isotropy of the lattice) for Ising interfaces in three dimensions.

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## Distribution of cycle lengths in spatial models of random permutations
<div align="center">DANIEL UELTSCHI</div>

This is a brief survey of models of random permutations that involve a spatial structure. Their common feature is a phase transition to a phase where infinite, macroscopic cycles are present. In addition, the cycle structure exhibits self-similarity, which results in Poisson-Dirichlet distributions.

**1. GEM and Poisson-Dirichlet measures.** Let us understand the self-similarity structure in a simple situation, random permutations with uniform distribution. Each permutation $\pi \in \mathcal{S}_n$ has probability $1/n!$. Let $\ell_1(\pi), \ell_2(\pi)$ be the lengths of the cycles of $\pi$, when ordered by the smaller index that belongs to the cycle. It is not hard to see that $\mathrm{Prob}(\ell_1 = k) = \frac{1}{n}$ for all $k = 1, \ldots, n$. It follows that, as $n \to \infty$,

- $\frac{\ell_1}{n} \to$ uniform random variable on $[0, 1]$;
- $(\frac{\ell_1}{n}, \frac{\ell_2}{n}, \ldots) \to \mathrm{GEM}(1)$.

The *Griffiths-Engen-McCloskey distribution* $\mathrm{GEM}(\theta)$ is the distribution for

$$\left( X_1, (1 - X_1)X_2, (1 - X_1)(1 - X_2)X_3, \ldots \right),$$

where $X_1, X_2, \ldots$ are i.i.d. beta random variables with parameter $\theta$; that is, $\mu(X_i > s) = (1 - s)^\theta$ for $0 \leq s \leq 1$. The *Poisson-Dirichlet distribution* $\mathrm{PD}(\theta)$ is the law obtained by rearranging the numbers above in decreasing order. See [10] for more information.

Let $\ell^{(1)}(\pi), \ell^{(2)}(\pi), \ldots$ be the cycle lengths in nonincreasing order. Then

$$\left( \frac{\ell^{(1)}}{n}, \frac{\ell^{(2)}}{n}, \ldots \right) \to \mathrm{PD}(1)$$

as $n \to \infty$. These laws are due to the self-similarity of cycle lengths.

**2. Random stirring model.** Consider a cubic box with $n$ sites in $\mathbb{Z}^d$. Random transpositions occur with i.i.d. exponential random variables with rate 1 at each edge. Let $\tau_1, \ldots, \tau_k$ be the transpositions that occur before time $t$, and let

$$\pi_t = \tau_k \circ \cdots \circ \tau_1$$

be the resulting permutation. At $t = 0$ we have $\tau_0 = \mathrm{id}$; for small $t$, $\pi_t$ looks very much like the identity, but with short cycles here and there. The cycle lengths typically grow over time, with the possibility that "infinite" cycles occur. We leave aside a proper definition of infinite cycles. We denote $\nu = \nu_t$ the fraction of sites that belong to infinite cycles.

**Conjecture.** Let $d \geq 3$. There exists $t_c$ such that
$$\nu = \begin{cases} 0 & \text{if } t < t_c, \\ > 0 & \text{if } t > t_c. \end{cases}$$
And when $\nu > 0$, the cycle structure is asymptotically given by
$$\left( \frac{\ell^{(1)}}{\nu n}, \frac{\ell^{(2)}}{\nu n}, \dots \right) \to \mathrm{PD}(1).$$

This models was introduced by Harris [11]. One can consider arbitrary graphs, and the version on trees was studied by Angel [2]. A beautiful result due to Schramm [14] is a variant of the conjecture above on the complete graph [14]; see Berestycki [3] for a nice and simpler (and partial) proof.

A similar model occurs as a representation for certain quantum spin systems. The distribution involves an extra $2^{\#\mathrm{cycles}}$. See [16, 1], and the recent survey of Ioffe [12]. The conjecture is that the cycle structure converges to the Poisson-Dirichlet distribution with parameter $\theta = 2$.

**3. Quenched model of spatial random permutations.** Choose positions $x_1, \dots, x_n$ in a box $\Lambda \subset \mathbb{R}^d$ according to a "suitable" point process, and define the probability of $\pi \in \mathcal{S}_n$ to be $\frac{1}{Z} e^{-H(\pi)}$, where the "Hamiltonian" is given by
$$H(\pi) = \sum_{i=1}^n \xi(x_i - x_{\pi(i)}).$$

The most relevant choice for the jump function is $\xi(x) = \frac{1}{4\beta} \|x\|^2$, where $\beta$ is a positive parameter (it represents the inverse temperature of the quantum Bose gas). One considers the limit where the size of the box and the number of points diverge, keeping the density $\rho = n/|\Lambda|$ fixed. This model was essentially introduced by Feynman [8]. Under restrictions on $\xi$, on $d$, and on the point process, one expects that the fraction $\nu$ of points in infinite cycles undergoes a transition.

**Conjecture.** There exists $\rho_c$ such that
$$\nu = \begin{cases} 0 & \text{if } \rho < \rho_c, \\ > 0 & \text{if } \rho > \rho_c. \end{cases}$$
And when $\nu > 0$, the cycle structure is asymptotically given by
$$\left( \frac{\ell^{(1)}}{\nu n}, \frac{\ell^{(2)}}{\nu n}, \dots \right) \to \mathrm{PD}(1).$$

This conjecture is supported by numerical simulations [9]. Let me also mention the unrelated but beautiful result of Biskup and Richthammer on the complete characterization of Gibbs states in the one-dimensional system [7].

**4. Annealed model of spatial random permutations.** This model is closely related to the quantum Bose gas, and it is also easier to study. The state space is $\Lambda^n \times \mathcal{S}_n$, where $\Lambda$ is a cubic box in $\mathbb{R}^d$. The expectation of a random variable $X$

is defined by

$$\mathbb{E}(X) = \frac{1}{Z} \int_{\Lambda^n} \mathrm{d}x_1 \dots \mathrm{d}x_n \sum_{\pi \in \mathcal{S}_n} X(\{x_i\}, \pi) \, \mathrm{e}^{-H(\{x_i\}, \pi)},$$

where $Z$ is the normalization, and the Hamiltonian is chosen of the form

$$H(\{x_i\}, \pi) = \sum_{i=1}^{n} \zeta(x_i - x_{\pi(i)}) + \sum_{\ell \geq 1} \alpha_\ell r_\ell(\pi).$$

Here, $\alpha_\ell$ are real parameters, and $r_\ell(\pi)$ denotes the number of $j$-cycles in $\pi$. In the case of the Bose gas, we have $\xi(x) = \frac{1}{4\beta}\|x\|^2$ and

$$\alpha_\ell = \frac{2\ell a}{(4\pi\beta)^{1/2}} \Big[ \tfrac{1}{2} \sum_{j=1}^{\ell-1} \Big( \frac{\ell}{j(\ell-j)} \Big)^{3/2} - \zeta(\tfrac{3}{2}) \Big] = -\frac{(6 - \gamma_{1/2})a}{\sqrt{4\pi\beta}} (1 + O(\ell^{-1/5})),$$

where $\gamma_{1/2} \approx 0.5396$ is a generalized Euler constant, and $a$ is the scattering length of the interaction potential between quantum particles. The calculation is exact but not rigorous and it can be found in [5]; its validity is not entirely clear.

We can give a rigorous characterization of the cycle structure under some assumptions. First, we suppose that the Fourier transform of $\mathrm{e}^{-\xi(x)}$ is nonnegative, and we denote it by $\mathrm{e}^{-\varepsilon(k)}$. Let us introduce the critical density $\rho_{\mathrm{c}}$ by the formula

$$\rho_{\mathrm{c}} = \sum_{\ell \geq 1} \mathrm{e}^{-\alpha_\ell} \int_{\mathbb{R}^d} \mathrm{e}^{-\ell\varepsilon(k)} \, \mathrm{d}k.$$

The result is essentially as stated in the next theorem. Some technicalities are left aside, and the interested reader is invited to consult Ref. [4] for the precise formulation.

> **Theorem.** Assume that $\alpha_\ell$ converges to some $\alpha \in \mathbb{R}$ as $\ell \to \infty$. The fraction of points in infinite cycles is then given by $\nu = \max(0, \frac{\rho - \rho_{\mathrm{c}}}{\rho})$. When $\nu > 0$, the cycle structure satisfies
> $$\Big( \frac{\ell^{(1)}}{\nu n}, \frac{\ell^{(2)}}{\nu n}, \dots \Big) \to \mathrm{PD}(\mathrm{e}^{-\alpha}).$$

This theorem was recently obtained with Betz [4]. It is based on results of Sütő for the ideal Bose gas [15]. It also uses estimates for weighted random permutations [13, 6]. In the case $\alpha_\ell = 1/\ell^\gamma$ with $\gamma > 0$, one can also prove that $\ell^{(1)}/\nu n \to 1$ in distribution, i.e. there is a single giant cycle above the critical density.

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## Kinetic coagulation models with particle fluxes.

Juan J. L. Velázquez

(joint work with M. Escobedo)

The classical coagulation equation reads:

$$
(1) \quad \partial_t f(x,t) = \frac{1}{2} \int_0^x K(x-y,y) f(x-y,t) f(y,t) \, dy - \int_0^\infty K(x,y) f(x,t) f(y,t) \, dy
$$

where $K(x,y) = K(y,x)$. This equation describes the aggregation of uncorrelated particles with sizes $x$, $y$ with the rate $K(x,y)$.

It is well known that the solutions of (1) exhibit the phenomenon called gelation for kernels $K(x,y) = (x \cdot y)^{\frac{\lambda}{2}}$, $1 < \lambda < 2$. This means that solutions of (1) globally defined in time do not preserve the mass $\int_0^\infty x f(x,t) \, dx$ even if they formally do so. The currently available theories of global solutions of (1) predict loss of mass after a finite time, but they do not describe the rate of loss of mass or the precise asymptotics of the solutions for large values of $x$.

We have developed a theory of classical solutions for (1) describing the solutions of (1) during the gelation regime. The obtained solutions behave asymptotically

for large values as:

$$f(x,t) \sim a(t) x^{-\frac{3+\lambda}{2}} \quad , \quad x \to \infty \quad , \quad a(t) > 0 \quad , \quad t \in [0,T]$$

The construction of the solutions is made by means of three different steps. The first step is a linearization argument around the solution $x^{-\frac{3+\lambda}{2}}$. This function is a stationary weak solution of (1) if a suitable concept of weak solutions is introduced. From the physical point of view this solution describes the continuous transfer of particles from $x = 0$ to $x = \infty$ with a constant flux at any point. The solutions of the linearized problem can be computed explicitly using Laplace transforms and the Wiener-Hopf method. This solution provides detailed information about the asymptotics of the solutions of the corresponding linearized problem. As a second step we study the linearization around an initial data $f_0(x)$ that behaves asymptotically as $Ax^{-\frac{3+\lambda}{2}}$ but it is globally bounded in $x$. This solution cannot be computed explicitly, but it can be obtained by means of a continuation argument that takes as starting point the explicit solution derived for the power law initial data. As a third step the solution of the nonlinear initial value problem (1) with initial data $f(x,0) = f_0(x)$ is obtained by means of a perturbative argument.

The solutions obtained in this manner have a flux of particles escaping towards the origin whose precise value depends on the initial distribution $f_0(x)$. The detailed constructions can be found in [3], [4], [5].

There are many analogies between the described construction of local solutions for (1) and a similar construction obtained for the Uehling-Uhlenbeck system in [1], [2]. One of the major differences, however, is the onset of some type of regularized effects for the solutions of (1) that are due to the fact that for large values of $x$ the operators that result linearizing (1) around $f_0$ behave, in suitably rescaled variables, to the half-derivative operator $D_x^{\frac{1}{2}}$.

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# On the singularities of a free boundary through Fourier expansion

Georg Sebastian Weiss

(joint work with J. Andersson, H. Shahgholian)

We are concerned with singular points of solutions to the *unstable* free boundary problem

$$\Delta u = -\chi_{\{u>0\}} \qquad \text{in } B_1.$$

The problem arises in applications such as solid combustion, composite membranes, climatology and fluid dynamics (see the references in [2]).

From [1] it is known that solutions to the above problem may exhibit singularities —that is points at which the second derivatives of the solution are unbounded— as well as degenerate points. This causes breakdown of by-now classical techniques. Here we introduce new ideas based on Fourier expansion of the nonlinearity $\chi_{\{u>0\}}$.

The method turns out to have enough momentum to accomplish a complete description of the structure of the singular set in $\mathbb{R}^3$.

A surprising fact in $\mathbb{R}^3$ is that although

$$\frac{u(r\mathbf{x})}{\sup_{B_1} |u(r\mathbf{x})|}$$

can converge at singularities to each of the harmonic polynomials

$$xy, \frac{x^2 + y^2}{2} - z^2 \text{ and } z^2 - \frac{x^2 + y^2}{2},$$

it may *not* converge to any of the non-axially-symmetric harmonic polynomials $\alpha\left((1+\delta)x^2 + (1-\delta)y^2 - 2z^2\right)$ with $\delta \neq 1/2$.

We also prove the existence of stable singularities in $\mathbb{R}^3$.

In contrast to the analysis of singularities for minimisers or stable solutions, where there are many methods available, there are few results on unique tangent cones at *unstable* singularities. Even the Lojasiewicz inequality approach (see for example [3]) would be hard to realize in our problem due to the lack of a suitable local Lyapunov functional; we do have a monotonicity formula playing the role of a local Lyapunov functional, but as it turns out it has the wrong scaling to be used at the unstable singularities of "supercharacteristic growth".

The natural approach would be to study blow-up limits in order to analyze the singularities. Unfortunately blow-up sequences of the type

$$\frac{u(r_j\mathbf{x} + \mathbf{x}^0)}{\sup_{B_{r_j}(\mathbf{x}^0)} |u|}$$

do not provide enough information of the solution as the nonlinearity of the equation vanishes in the limit. To preserve some information of the nonlinearity we

consider

$$(1) \qquad \frac{u(r_j\mathbf{x} + \mathbf{x}^0)}{r_j^2} - \Pi(u, r_j, \mathbf{x}^0),$$

where $\Pi(u, r_j, \mathbf{x}^0)$ is a suitable projection of $u(r_j\mathbf{x} + \mathbf{x}^0)/r_j^2$ in $B_1$ onto the homogeneous harmonic second order polynomials.

It can be shown that if

$$\lim_{j\to\infty} \frac{u(r_j\mathbf{x} + \mathbf{x}^0)}{\sup_{B_{r_j}(\mathbf{x}^0)} |u|} = p(\mathbf{x}),$$

then

$$\lim_{j\to\infty} \left( \frac{u(r_j\mathbf{x} + \mathbf{x}^0)}{r_j^2} - \Pi(u, r_j, \mathbf{x}^0) \right) = Z_p,$$

where $Z_p$ is a solution of

$$\Delta Z_p = -\chi_{\{p>0\}}.$$

Next we notice that, at each singular point $\mathbf{x}^0$,

$$\lim_{j\to\infty} \frac{\Pi(u, r_j, \mathbf{x}^0)}{\sup_{B_1} |\Pi(u, r_j, \mathbf{x}^0)|} = \lim_{j\to\infty} \frac{u(r_j\mathbf{x} + \mathbf{x}^0)}{\sup_{B_{r_j}(\mathbf{x}^0)} |u|}.$$

So in order to prove uniqueness of $p$ it is sufficient to control how $\Pi(u, r, \mathbf{x}^0)$ changes when $r$ varies. More precisely we would want to estimate

$$(2) \qquad \left| \frac{\Pi(u, r, \mathbf{x}^0)}{\sup_{B_1} |\Pi(u, r, \mathbf{x}^0)|} - \frac{\Pi(u, r/2, \mathbf{x}^0)}{\sup_{B_1} |\Pi(u, r/2, \mathbf{x}^0)|} \right|.$$

Our method of proof is based on the observation that $u(r\mathbf{x} + \mathbf{x}^0) \approx \tau_r p_r + Z_{p_r}$ in $B_r$, where $p_r$ is a second order harmonic polynomial of norm 1. It follows that $\Pi(u, r/2, \mathbf{x}^0) \approx \Pi(\tau_r p_r + Z_{p_r}, 1/2, 0) = \Pi(\tau_r p_r, 1/2, 0) + \Pi(Z_{p_r}, 1/2, 0) = \tau_r p_r + \Pi(Z_{p_r}, 1/2, 0)$. Therefore it is essential to control $\Pi(Z_{p_r}, \cdot)$ in order to estimate (2). This control is achieved by means of an explicit calculation of the Fourier coefficients of $Z_{p_r}$.

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## A functional analytic approach to logarithmic Sobolev inequalities and the hydrodynamic limit

Maria G. Westdickenberg

(joint work with Natalie Grunewald, Felix Otto, Cédric Villani)

The logarithmic Sobolev inequality (LSI) is a powerful tool for studying convergence to equilibrium in spin systems. The Bakry-Emery criterion implies LSI in the case of a convex Hamiltonian. What can be said in the nonconvex case? We present two recently developed sufficient conditions for LSI. The first is a Bakry-Emery-type criterion that requires only LSI (not convexity) for the single-site conditional measures. The second is a two-scale condition: An LSI on the microscopic scale (conditional measures) and an LSI on the macroscopic scale (marginal measure) are combined to prove a global LSI. Continuing in the spirit of the two-scale approach, we also present a two-scale criterion for the hydrodynamic limit and explain how it can be applied in the context of the Guo-Papanicolaou-Varadhan example.

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