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# PDE and Materials

Organised by
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ABSTRACT. This meeting brought together a carefully selected group of mathematicians, physicists, material scientists and engineers to discuss and review the impact of modern mathematical methods on the understanding of material behaviour and the design of new materials. A key issue is that the material behaviour is determined by physical processes at many different spatial and temporal scales which cannot be simultaneously resolved by brute force computation. Central themes of the meeting were (spatial) microstructures, the relation between atomistic and continuum models, the treatment of multiple temporal scales, and the influence of randomness and the use of methods from statistical mechanics.

## Introduction by the Organisers

This meeting brought together a carefully selected group of mathematicians, physicists, material scientists and engineers to discuss and review the impact of modern mathematical methods on the understanding of material behaviour and the design of new materials. A key issue is that the material behaviour is determined by physical processes at many different spatial and temporal scales which cannot be simultaneously resolved by brute force computation. There are a number of heuristic approaches (such as the quasicontinuum method or accelerated dynamics) to address the multiscale problem, but a mathematical theory which allows one to understand when and it what sense these approaches provide a good approximation to the full problem is still in its infancy.

Central themes of the meeting were (spatial) microstructures, the relation between atomistic and continuum models, the treatment of multiple temporal scales,

and the influence of randomness and the use of methods from statistical mechanics. The recent theory of microstructures in crystalline materials which undergo solid-solid phase transitions has lead to a very inspiring bridge between materials science and the mathematical analysis of regularity and of oscillations in nonlinear partial differential equations, in particular the theory of compensated compactness by F. Murat and L. Tartar. At the meeting L. Székelyhidi presented a recent breakthrough in this area, a characterization of all compact sets in the space of $2 \times 2$ matrices which support a nontrivial microstructure. Other important contributions include new regularity results by C. Melcher and the use of new rigidity estimates and topological constructions to derive theories of lower-dimensional elastic objects (G. Dolzmann). Regularizations, e.g., due to interfacial energies or strain-gradient terms in elasticity or exchange energy terms in magnetic materials, prevent the formation of the mathematically idealized infinitely fine microstructures and break the dilation invariance of the problem by introducing a length scale. Interestingly this single additional scale can lead to the formation of complex patterns on a multitude of scales ('domain branching') and S. Conti presented interesting new results for type-I superconductors, based on subtle interpolation inequalities. In a different direction J.M. Robbins showed how the control of topological singularities through the shape of the container might lead to new switching mechanics for liquid crystals. E. Salje presented new experimental data and theoretical analyses on the interaction between mechanical microstructure and chemical behaviour and E. Quandt showed how the evolution of domain structures in magnetostrictive devices influences the performance of engineering devices.

The connection between atomistic and continuum models is mathematically at its very beginning, not the least because the powerful theory of pde and the calculus of variations at the continuum level has so far no equally powerful counterpart for discrete systems. C. Ortner presented first results from his PhD thesis for a one-dimensional numerical analysis of the quasicontinuum method, a numerical scheme which tries to switch adaptively between continuum and atomistic models. G. Friesecke showed how a rigorous analysis of screening effects leads to a linear scaling of the energy with the number of atoms ('stability of matter'). F. Theil presented a new approach to derive the Boltzmann equation from a discrete model of interacting atoms (without recollisions). This was closely related to an inspiring lecture by O. Penrose on the relation between microscopic reversibility and macroscopic irreversibility, which sparked a very lively discussion. More generally new rigorous results in statistical mechanics (the oldest multiscale method) played a key role at the meeting, notably in the talks by E. Presutti and R. Kotecký. S. Luckhaus presented a new model Hamiltonian that can serve as a starting point for a statistical mechanics of solids, including a description of defects, such as dislocations or grain boundaries. The influence of randonmess and heterogeneity on the behaviour at macroscopical scales was analyzed in the talks by N. Dirr, G. Menon, B. Niethammer and A. Planes.

The strong separation of time scales is one of the major bottlenecks in the use of molecular dynamics simulations. Indeed often the processes which are most interesting from the point of view of applications in chemistry, physics and biology occur at times scales which are well beyond any MD simulation with realistic potentials. The organized a special session to contrast some of the current approaches in the mathematics, physics and computational communities (C. Schütte, E. Vanden-Eijnden, A. Voter). This was complemented by A. Mielke's rigorous analysis of two-scale Hamiltonian systems and M. Ortiz new approach to microstructure evolution by a global minimization principle in space-time. In addition to the lectures the very special environment of Oberwolfach provided an excellent opportunity for informal discussions, allowing for an open exchange of ideas between people which usually attend separate groups of conferences.

# Workshop: PDE and Materials

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# Abstracts

### First order phase transitions in particles models with spins
Errico Presutti

My talk is based on a research I am doing in collaboration with A. De Masi, I. Merola and Y. Vignaud. The ultimate goal of my research project is to understand nature and structure of phase transitions in systems of particles in the $d$-dimensional Euclidean space $\mathbb{R}^d$. A breakthrough in this program was the work with J.L. Lebowitz and A. Mazel, [1], where a system of identical point particles in $\mathbb{R}^d$ interacting via Kac-like potentials was shown to exhibit a liquid-vapor phase transition. The next step in my program is now to extend the analysis to systems where particles have spins and the interaction depends on the spins as well. One may then expect the emergence of spatial patterns and the hope is to start in this way the investigation of crystals like structures. This is unfortunately still far from what I am able to accomplish but what I am reporting here is a maybe short yet still a step in this direction.

As the audience may be more familiar with functionals and variational problems, I will first present the "mesoscopic" version of the model and then briefly state how the results extend to the true particle system. Thus the free energy functional I am considering, which may be called the continuum Potts free energy functional, is a functional on the space $L^\infty(\mathbb{T}, \mathbb{R}_+)^S$, $S \geq 2$, $\mathbb{T}$ a torus in $\mathbb{R}^d$, $d \geq 2$, defined by

$$(1) \qquad F(\rho_1, .., \rho_S) = \frac{1}{2} \sum_{s \neq s'} \langle J\rho_s, J\rho_{s'} \rangle - \sum_s \{\lambda \langle \rho_s, 1 \rangle + \frac{1}{\beta} \langle I(\rho_s), 1 \rangle\}$$

where $\langle f, g \rangle = \int_{\mathbb{T}} f(r)g(r)$ is the $L^2$ scalar product in $\mathbb{T}$; $J = J(r, r')$ is a smooth, symmetric, probability kernel such that $J(r, r') = J(0, r' - r)$ and $J(0, r) = 0$ if $|r| \geq 1/2$. $\lambda \in \mathbb{R}$ is the chemical potential, $\beta > 0$ the inverse temperature, $I(\rho) = -\rho(\log \rho - 1)$ the entropy and $\rho_s$, $s \in \{1, .., S\}$, the density of particles with spin $s$.

In the mesoscopic theory the thermodynamic free energy density is

$$(2) \qquad f_{\beta,\lambda} = \lim_{\mathbb{T} \nearrow \mathbb{R}^d} \frac{1}{|\mathbb{T}|} \inf_{\rho_1, .., \rho_S} F(\rho_1, .., \rho_S)$$

and the pure phases are the minimizers (in the limit as $\mathbb{T} \nearrow \mathbb{R}^d$). Thus a phase transition corresponds to the existence of more than one minimizer.

**Proposition 1.** *For any torus $\mathbb{T}$ the inf of $F(\rho_1, .., \rho_S)$ is attained on functions $\rho_1, .., \rho_S$ which are all constant on $\mathbb{T}$. Consequently*

$$(3) \qquad f_{\beta,\lambda} = \inf_{x_1, .., x_S \in \mathbb{R}_+^S} \frac{1}{2} \sum_{s \neq s'} x_s x_{s'} - \sum_s \{\lambda x_s + \frac{1}{\beta} I(x_s)\}$$

The proof of Proposition 1 is based on changing $\rho_s \to J\rho_s$ and to exploit a convexity inequality for the difference $\langle JI(\rho_s) - I(J\rho_s), 1 \rangle \}$. The variational problem (3) has been studied analytically, but some steps are only established numerically, so that at the moment I have not a complete proof of the following proposition (whose validity however is established analytically for large $S$).

**Proposition 2.** *There exists a smooth curve $\lambda = \lambda(\beta)$ such that if $\lambda < \lambda(\beta)$ then there is a unique minimizer $x^{\mathrm{dis}} = (x_1^{\mathrm{dis}}, .., x_S^{\mathrm{dis}})$ of (3) and $x_1^{\mathrm{dis}} = .. = x_S^{\mathrm{dis}}$. If instead $\lambda > \lambda(\beta)$ there are $S$ minimizers, one is $x_1^{\mathrm{ord}} = .. = x_{S-1}^{\mathrm{ord}} < x_S^{\mathrm{ord}}$ the others are obtained by a permutation of labels.*

*At $\lambda = \lambda(\beta)$ and $d = 2$ there is a unique minimizer $x^{\mathrm{dis}} = (x_1^{\mathrm{dis}}, .., x_S^{\mathrm{dis}})$ while for $d > 2$ there are $S+1$ minimizers, one is $x^{\mathrm{dis}}$ the others are $x_1^{\mathrm{ord}} = .. = x_{S-1}^{\mathrm{ord}} < x_S^{\mathrm{ord}}$ and its permutations.*

*The total density $X(\lambda, \beta) = x_1 + \cdots + x_S$, $(x_1, .., x_S)$ a minimizer of (3), is then well defined for any $\lambda \neq \lambda(\beta)$. $X(\lambda, \beta)$ is an increasing function of $\lambda$ and in $d \geq 3$, $X(\lambda, \beta)$ jumps at $\lambda = \lambda(\beta)$.*

Thus at the critical point in $d \geq 3$ there is a phase transition which persists also if we are "color blind" namely if we ignore the values of the spins (identified here with colors). Indeed at the critical point the disordered state has a total density strictly smaller than that of the ordered state. In other words the typical distance among particles in the ordered state is strictly smaller than in the disordered one, and since the ordered state has a non zero magnetization, the appearance of a spontaneous magnetization comes together with a restriction of the inter-particles distances, a phenomenon observed in ferromagnetic crystals and known as magnetostriction. See [2] for an analysis of the phenomenon in a lattice model.

The particle Hamiltonian $H_\gamma(q)$, $q = \{q^{(1)}, .., q^{(S)}\}$, $q^{(s)} = (..., q_{i-1}^{(s)}, q_i^{(s)}, q_{i+1}^{(s)}, ...)$, $q_i^{(s)} \in \mathbb{R}^d$, which corresponds to the free energy (1), is

$$(4) \qquad H_\gamma(q) = \frac{1}{2} \sum_{s \neq s'} \langle J_\gamma * q^{(s)}, J_\gamma * q^{(s')} \rangle - \lambda \sum_s |q^{(s)}|, \quad J_\gamma(r, r') = \gamma^d J(\gamma r, \gamma r')$$

$|q^{(s)}|$ the total number of elements of $q^{(s)}$ (supposed finite for each $s$). $\gamma > 0$ is the Kac scaling parameter and the scaling $r \to \gamma r$ moves from the microscopic to mesoscopic levels, we should thus think that $\gamma$ is a small parameter. The original results by Kac, Lebowitz and Penrose showed that in a large class of models in the limit as $\gamma \to 0$ Gibbsian statistical mechanics reproduces the van der Waals theory. The emphasis in this talk is that I want $\gamma > 0$ maybe small yet fixed, so that the system is a genuine model of statistical mechanics with finite range interactions and phase transitions are the phase transitions of the DLR theory.

**Theorem 3.** *Let $d \geq 3$ and $\beta > 0$. Then there exists $\gamma_\beta > 0$ and for any $\gamma \leq \gamma_\beta$ a chemical potential $\lambda(\beta, \gamma)$ so that at $\beta, \lambda(\beta, \gamma)$ there are $S + 1$ distinct extremal*

*DLR measures. Their average densities converge as $\gamma \to 0$ to the minimizers of the mesoscopic model, as described in Proposition 2.*

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## Disorder in magnetic and martensitic transitions: hysteresis, metastability and avalanches

ANTONI PLANES

(joint work with Eduard Vives, Teresa Castán and Lluís Mañosa)

First-order phase transitions are expected to occur abruptly at given values of external control parameters such as temperature, pressure or applied field (stress, magnetic or electric). In solid materials, however, they rarely show such an ideal behaviour. Commonly, the expected sharp change of the order parameter is smoothed out and thus the transition spreads over a certain range of the external control parameter. Moreover, in a number of systems the transition is even preceded by anomalies, typically detected in the response to certain excitations, which may arise from local symmetry breaking perturbations [1]. Systems undergoing magnetic and martensitic transitions are typical examples where this behaviour is observed. Actually, it is accepted that the influence of disorder in the form of randomly quenched defects, deviations from stoichiometry, impurities, etc..., always present in any solid system, is at the origin of all these deviations with respect to the ideal behaviour. On the one side, this is due to the fact that these systems sensitively respond to disorder by, for instance, giving rise to variations of the effective local transition temperature. On the other side, as already pointed out by Imry and Wortis [2], disorder blocks the growth of the correlations when the transition starts. The most evident consequence of these features is the existence of an extended region where the high and low symmetry phases coexist. The transitions to be considered are thus associated with the existence of high energy barriers which separate the two phases that must be overcome for the transition to proceed. Indeed, in the coexistence region the actual state of the system is metastable and history dependent [3].

The following features are characteristic of such *extended* first-order phase transitions.
(i) The existence of long range forces of elastic or magnetic nature, arising from compatibility conditions (or dipolar forces) associated with the system boundaries and/or interfaces [4]. The external force driving the transition must then compete with the whole system and not only with a small microscopic domain. Thus thermal fluctuations play, in general, only a minor role, which means that the time scale of the thermal activation processes $\tau_{\mathrm{th}}$ (which depends on temperature and

on the effective height of the energy barriers) is typically very large compared to the time scale $\tau_{\mathrm{dr}}$ associated with the driving field. The transition kinetics shows therefore, an athermal character.

(ii) Energy barriers are inhomogeneously distributed in the system. This gives rise to the existence of a complex energy landscape with multiple energy minima. Any modification of the amount and spatial distribution of disorder affects this energy landscape and may thus strongly modify the transition path. In some cases this can be achieved by cycling through the transition. In martensitic systems, cycling enables to establish an optimal transition path that avoids high energy barriers.

(iii) Within a broad range of driving rates, the response of the system to the driving parameter shows an avalanche behaviour [5]. Different experimental detection techniques reveal that the evolution of the transition is characterized by burst-like events separated by inactivity periods. Such events correspond to jumps from one metastable state to another involving dissipation of energy. In many cases the properties of the avalanches reveal a lack of characteristic scales within a broad range of time, sizes and energies. Although this makes it difficult to properly define a characteristic time scale associated with the avalanches, the duration of the longest detected avalanche event $\tau_{\mathrm{av}}$ is typically much smaller than the time scales associated with thermal activation processes $\tau_{\mathrm{th}}$. If $\tau_{\mathrm{av}} \ll \tau_{\mathrm{dr}}$ is also satisfied, the system behaves rate independent.

The prototypical model for understanding avalanche behaviour in first-order athermal phase transitions is the Random Field Ising Model with $T = 0$ metastable dynamics [6]. This is a lattice model with spin variables $S_i$ (which can represent domains or small regions of the material) localized on each lattice site and coupled ferromagnetically. Quenched Gaussian random fields with zero mean and standard deviation $\sigma$ are defined on each site. They represent the effect of disorder. The model is subjected to an external field. When the system is driven starting from a very high value of the field $H$, the saturated state with all $S_i = +1$ evolves following a deterministic dynamics consisting of a local energy relaxation of single spins. Once a spin flips, this may trigger flipping of neighbouring spins and thus an avalanche initiates. During avalanches the driving field is kept constant until a new metastable situation is reached. This kinetics conveniently mimics athermal dynamics in real systems and corresponds to a situation of rate independent hysteresis.

By numerical simulations one obtains hysteresis loops consisting of a sequence of avalanches joining metastable states. These avalanches are in general microscopic which means that in the thermodynamic limit, the associated jumps involve the transformation of a vanishingly small fraction of the system. Interestingly, the loops exhibit a transition from being smooth when $\sigma > \sigma_c$ to showing a ferromagnetic macroscopic discontinuity when $\sigma < \sigma_c$. At $\sigma_c$ the distribution of avalanches is critical and can be characterized by a well defined exponent. Other similar models, including random bonds, random anisotropy, etc. have also been studied [7]. They all display similar behaviour and it has been shown that the critical exponents exhibit a high degree of universality [8].

These results suggest the existence of a disorder-induced phase transition in the hysteresis loop. Only few experimental works have been designed to experimentally corroborate its actual existence. The difficulty arises from the possibility of controlling the amount of disorder in a given system. Two works are worth mentioning. On one side, Berger at al. [9] studied the effect of magnetic disorder on the magnetization reversal process in Co/CoO bilayers. In this case, the ferromagnetic Co layer is coupled to the antiferromagnetic CoO which allows a reversible tuning of disorder by temperature variation from above to below its Néel point. In another work, Marcos et al. [10] reported measurements in the magnetically glassy phase of Cu-Al-Mn alloys. In this case, due to coexistence of ferromagnetic and antiferromagnetic components in the system, temperature changes enable to modify the effective disorder causing the disorder-induced transition. Critical exponents have been obtained from scaling analysis of the hysteresis loops. The values reported for the two systems are in quite good agreement but show some disagreement with critical exponents corresponding to lattice models. This indicates that even though $T = 0$ lattice models reveal that disorder is the essential feature which enables a satisfactory understanding of the scenario described above, they lack some important physical ingredient necessary to account for finite temperature measurements.

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## Interfaces in a Heterogeneous Environment
### Nicolas Dirr

**1. Introduction** In the classical continuum mechanics approach materials are described by conservation laws and constitutive relations. As both are given on the continuum scale, not on the atomistic scale, they are necessarily relations between *averaged* quantities.

The qualitative understanding of materials at nonzero temperature in an inhomogeneous environment will be improved by taking into account fluctuations around this average that may arise from thermal effects or from impurities of the environment. The origin of these fluctuations are stochastic effects on the atomistic level, hence an approach considering several scales is often necessary.

I present several rigorous mathematical results for models for interfaces under the influence of random or periodic perturbations on several spatial and temporal scales. The models under consideration capture the interplay of

- the interfacial energy;
- time-independent random and/or deterministic inhomogeneities on a very small spatial scale;
- space-time dependent noise, modelling thermal fluctuations.

I present results both for the effective energy on a large scale and for the dynamics of such models. The dynamical models under consideration are in the over-damped limit, informally speaking, this means inertial effects are neglected, the system is driven by energy dissipation, and therefore only first derivatives in time are considered.

**2. Effective interfacial energy for a mesoscopic random functional** (Joint work with Enza Orlandi, Roma III)

A model for an energy on a so-called mesoscopic scale where the quenched random structure of the environment and the interfacial energy compete is the following functional:

$$G_\epsilon(u) := \int_\Omega \left[ \epsilon |\nabla u|^2 + \frac{W(u)}{\epsilon} + \frac{\theta(\epsilon)}{\epsilon} g_\epsilon(x, \omega) u \right] dx,$$

$g_\epsilon$ is a random field bounded in $L^\infty$ with correlation length $\epsilon$ and mean zero, and $W$ is a double-well potential with minima $\pm 1$. The limit $\epsilon \to 0$ corresponds to the transition from the meso- to the macroscale and yields an effective surface energy. Note that minimisers are not spatially constant, hence the minimal energy is negative and may, as $\epsilon \to 0$, diverge to $-\infty$, so we consider

$$F_\epsilon(u) = G_\epsilon(u) - \left( \inf_{H^1(\Omega)} G_\epsilon(\cdot) \right)$$

We show for $\theta$ nonnegative and sufficiently small, but not necessarily vanishing as $\epsilon \to 0$, that the energy is bounded from below by a suitably coarse-grained energy that depends only on the averages of $u$ in cubes of sidelength $\epsilon$. (Contour reduction)

In the special case $\theta(\epsilon) \sim [\log(1/\epsilon)]^{-1}$ we show the $\Gamma$-convergence of $F_\epsilon$ to a constant multiple of the interface are. The case of small but finite $\theta$ is work in progress, while the case of a periodic environment was considered in a joint paper with M. Lucia and M. Novaga, see [2].

**3. Pulsating Waves for Interfaces in a Periodic Environment** (Joint work with Nung Kwan Yip.) We consider an interface in a periodic environment, evolving by forced mean curvature flow, i.e. $V_X = \kappa_X + f(X) + F$, where $V_X$ is the normal velocity and $\kappa_X$ the mean curvature of the interface at a point $X \in \mathbb{R}^{n+1}$. $F$ is a constant "field" that "drives" the interface through the "obstacles" which are given by $f(X)$. We assume that the interface has the form $(x, u(x,t))$, $x \in \mathbb{R}^n$, $u(x,t) \in \mathbb{R}$, i.e. a graph over a coordinate plane, and we make for small gradients the following (heuristic) approximation of the equation:

(1) $$u_t = \Delta u + f(x, u) + F, \quad u(x,t) \text{ periodic in } x,$$

$f(\cdot, \cdot)$ is 1-periodic in *both* variables, bounded, mean zero, and $F \geq 0$. We show (see [3]): There exists $F_* > 0$ such that for any $0 \leq F \leq F_*$ there exists a periodic stationary solution of (1), called *pinning state*, while for $F > F_*$, there exist *pulsating wave solutions* $U_F(x,t)$ with velocity $V_F$ :

$$U_F(\cdot, t + 1/V_F) = U_F(\cdot, t) + 1.$$

For a large class of $f(x,u)$ we determine the scaling of the velocity of the pulsating wave near the critical forcing and obtain $V_F \sim A[(F - F_*)_+]^{\frac{1}{2}}$, for details see [3].

If the periodic forcing is sufficiently weak, a curve which is a graph stays a graph under forced mean curvature flow, and the qualitative behaviour is the same as that of the approximation considered above. This result and the construction of pulsating waves for equation (1) with linear growth will be contained in a forthcoming paper with Georgia Karali and Nung Kwan Yip.

**4. Switching for Ising spins with Kac potential** (Joint work with Giovanni Bellettini, Anna De Masi and Errico Presutti)

Here we consider a model where the environment is homogeneous, but there is an interplay of interfacial energy and thermal fluctuations. We consider a family of random variables on a lattice (spins) which take values in $\{-1, 1\}$ and which "flip," i.e. change their sign, according to the average of their neighbours in a large region (Kac-interaction). The interaction is constructed in such a way that a spin prefers to have the same sign as the average of the neighbours (ferromagnetic).

Ising models with Glauber dynamics (non-conserved order parameter) and Kac interaction have the property that their distribution is close to a product measure, therefore the coarse-grained spins converge on the mesoscale (space rescaled with interaction range, time unscaled) to the solution of a (deterministic) nonlocal evolution equation. The solutions of this equation can be described as being close to either one of two stable equilibria, separated by a transition layer. Under diffusive rescaling, i.e. on the macroscale, in the so-called sharp interface limit, the evolution of this transition layer is described by mean curvature flow. We

study the effect of the deviations of the underlying random process from the limit evolution on the meso-and macroscale, the *dynamic large deviations.*

We study a variational problem formulated in terms of a functional which approximates the rate function for large deviations in Ising systems with Glauber dynamics and Kac potentials. The spatial domain is $Q_L = [-L/2, L/2]^n$, $n = 2$ or $n = 3$, for $L \gg 1$. The action functional

$$I_{L;T}(m) = \frac{1}{4} \int_0^T \int_{Q_L} \left[ m_t + \frac{\delta F(m)}{\delta m} \right]^2 dx\,dt$$

is to be minimised under the constraint that the system switches from the negative stable equilibrium $(m(x) = -m_\beta)$ to the positive stable equilibrium, i.e. the infimum is taken over the set

$$\mathcal{U}_{L,T} = \{ m \in C^\infty(Q_L \times [0,T]) : m(r,0) = -m_\beta,\ m(r,T) = m_\beta, \}$$

and then the infimum over the the time $T > 0$ is taken (no time constraint). Here $F(m)$ is the mesoscopic free energy

$$F(m) = \int_{Q_L} \phi_\beta(m)\,dx + \frac{1}{4} \int_{Q_L \times Q_L} J(x, x')[m(x) - m(x')]^2 dx\,dx',$$

where $J$ is a smooth nonnegative kernel which takes into accout reflecting (Neumann) boundary conditions, and $\phi_\beta(m)$ a double-well potential. The action is zero for paths which follow the $L^2$-gradient flow of $F(m)$. (This is slightly different for the actual spin system.)

For $L$ large enough the penalty for tunnelling from the minus to the plus equilibrium states is determined. Minimising sequences are fully characterised and shown to have approximately a planar symmetry at all times, thus departing from the Wulff shape in the initial and final stages of the tunnelling. For details see [1].

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## Energy scaling and domain branching in type-I superconductors

Sergio Conti

(joint work with Rustum Choksi, Robert V. Kohn, Felix Otto)

The intermediate state of type-I superconductors is a classical pattern-formation problems in physics, first studied by Landau in the 30s [15, 16]. Similar patterns were discussed for magnetic domains by Lifshitz in 1944 [17], and later by Hubert [11]. The first mathematical results in this direction have been obtained by Kohn and Müller in 1992-1994 [13, 14] for the case of shape-memory alloys.

Their work originated a large amount of mathematical investigations of related pattern-formation problems in materials; for example, similar domain branching has been demonstrated in models of uniaxial ferromagnets [4, 5], thin-film blistering [12, 1], diblock copolymers [2], and dislocation walls in crystal plasticity [9]. Asymptotic self-similarity of the minima was proven, for a simplified version of the Kohn-Müller model, in [7].

The mathematical study of the type-I superconductors problem via energy minimization was begun by Choksi, Kohn and Otto in [6], leading to the derivation of four different rigorous upper bounds for the ground state energy, one of which was obtained through to a new two-scale flux-branching construction. This shows in particular that the picture previously obtained by heuristic means was incomplete. A first lower bound for intermediate fields was also obtained in [6]. We completed in [3] the analysis by providing matching lower bounds, thereby proving that exactly those different regimes are traversed with increasing magnetic field.

The functional we consider is, after scaling and elimination of the mean-field term,

$$E(B,\chi) = \int_\Omega \left[ B_2^2 + B_3^2 + (1-\chi)(B_1-1)^2 \right] \, dx \, dy \, dz$$

$$+ \, \varepsilon \int_\Omega |\nabla \chi| \, + \int_{\mathbb{R} \times \mathbb{T}^2 \setminus \Omega} |B - b_a|^2 \, dx \, dy \, dz.$$

Here $\Omega = (0,L) \times \mathbb{T}^2$, where $\mathbb{T}^2$ denotes the two-dimensional torus, identified with the unit square $Q = (0,1)^2$ with periodic boundary conditions; $B \in L^2_{loc}(\mathbb{R} \times \mathbb{T}^2, \mathbb{R}^3)$ and $\chi \in BV((0,L) \times \mathbb{T}^2, \{0,1\})$. The small parameter $\varepsilon > 0$ represents the surface energy for the normal-superconducting interfaces, and $b_a = (b_a, 0, 0)$ is the applied magnetic field, in units of the saturation field. Further, the fields satisfy $B\chi = 0$ a.e., representing the Meissner effect, and $\operatorname{div} B = 0$ distributionally, from Maxwell's equations. A full description of the energy and of its physical motivation can be found in [6].

**Theorem 1** (Lower bound from [3]; upper bound from [6])**.** *There exists a constant $c$ such that for all $b_a \in (0,1)$, and all $\varepsilon$ sufficiently small, we have*

$$\frac{1}{c} f\left(\varepsilon, L, b_a\right) \leq \inf E(B,\chi) \leq c f\left(\varepsilon, L, b_a\right),$$

*where the infimum is taken over all $\mathbb{T}$-periodic fields $B$ and $\chi$ which fulfill the compatibility conditions $\operatorname{div} B = 0$ distributionally and $B\chi = 0$ a.e.. Here*

$$f(\varepsilon, L, b_a) = \begin{cases} b_a \, \varepsilon^{4/7} \, L^{3/7} & \text{if } b_a \leq (\varepsilon/L)^{2/7} \leq 1/2 \\ b_a^{2/3} \, \varepsilon^{2/3} \, L^{1/3} & \text{if } (\varepsilon/L)^{2/7} \leq b_a \leq 1/2 \\ (1-b_a)|\ln(1-b_a)|^{1/3} \varepsilon^{2/3} L^{1/3} & \\ & \text{if } (\varepsilon/L)^{2/3} \leq \dfrac{(1-b_a)}{|\ln(1-b_a)|^{1/3}} \, , b_a > 1/2 \\ (1-b_a)^2 L & \text{otherwise.} \end{cases}$$

The proof is based on estimating the normal component $B_1$ in appropriate negative norms. For example, the last term in the energy gives directly an estimate on the $H^{-1/2}$ norm of $B_1(0, \cdot, \cdot) - b_a$. In turn, the difference $B_1(x_1, \cdot, \cdot) - B_1(0, \cdot, \cdot)$ can be estimated by testing with some $\psi : \mathbb{T} \to \mathbb{R}$ and computing

$$
\begin{aligned}
\int_{\mathbb{T}} (B_1(x_1, \cdot) - B_1(0, \cdot)) \, \psi(y, z) &= \int_{\mathbb{T}} \int_0^{x_1} \frac{\partial B_1}{\partial x}(x, y, z) \, \psi(y, z) \, dx \, dy \, dz \\
&= -\int_{\mathbb{T}} \int_0^{x_1} (\nabla' \cdot B') \, \psi \, dx \, dy \, dz \\
&= \int_{\mathbb{T}} \int_0^{x_1} B' \cdot \nabla' \psi \, dx \, dy \, dz \\
&\leq \|\nabla \psi\|_{L^\infty(\mathbb{T})} \int_{\mathbb{T}} \int_0^{x_1} (1 - \chi) |B'| dx \, dy \, dz \\
&\leq \|\nabla \psi\|_{L^\infty(\mathbb{T})} \|1 - \chi\|_{L^2(\Omega)} \|B'\|_{L^2(\Omega)} \,.
\end{aligned}
$$

Here we used first $\operatorname{div} B = 0$, integrated by parts, and then $B\chi = 0$. The result corresponds to an estimate of the Monge-Kantorovich, or $W^{-1,1}$ norm of $B_1(x_1, \cdot) - B_1(0, \cdot)$. At the same time one can relate $B_1(x_1, \cdot)$ to $\chi(x_1, \cdot)$.

Finally, the argument is concluded by constructing a good test function $\psi$, to be inserted in the previous estimates, which reproduces the structure of $\chi(x_1, \cdot)$ but is smoother. The key ingredient is given in the following Lemma, which was first used in a different context in [8]. Briefly, this states that if $|\nabla \chi|$ is small then the support of $\chi$ can be well approximated with a regular set, on which a significant part of the volume must concentrate. We thank Stephan Luckhaus and Francesco Maggi for pointing out to us that De Giorgi had used a very similar covering in proving compactness of sets of finite perimeter [10, Lemma II].

**Lemma 1** (From [8, 3]). *Let $S \subset \mathbb{T}$ be a set of finite perimeter, and let $\ell > 0$ be such that*

$$\ell \operatorname{Per}(S) \leq \frac{1}{4}|S| \,.$$

*Then there exists a finite union of balls $S_\ell \subset \mathbb{T}$ with the properties*

   (i) $|S \cap S_\ell| \geq \frac{1}{2}|S|$.
   (ii) $S_\ell = \bigcup_{i=1}^k B_\ell(x_i)$, where $k \leq c|S|/\ell^2$.

The Lemma is used with $S = \{p \in \mathbb{T} : \chi(x_1, p) = 1\}$ for a suitably-chosen $x_1 \in (0, L)$. One then fixes a parameter $r > 0$, which corresponds to the opening of the flux tubes on the surface, and defines a test function $\psi : \mathbb{T} \to \mathbb{R}$ by

$$\psi(p) = \max \{r - \operatorname{dist}(p, S_\ell) ; 0\} \,,$$

The estimates above in negative spaces give an upper bound on $\int_{\mathbb{T}} B_1(x_1, \cdot) \psi$ in terms of the energy. At the same time, (i) of Lemma 1 shows that $\int_{\mathbb{T}} \chi \psi$ is bounded from below by $r|S| \sim r b_a$. A careful choice of the parameters $r$ and $\ell$ permits then to prove the lower bounds. Details are given in [3].

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## Regularizations of mean-field models for Ostwald ripening

Barbara Niethammer

(joint work with J. Velázquez)

We consider the late stage coarsening of second phase particles in a first order phase transition where the particles interact by diffusional mass exchange to reduce their total surface area. The classical theory by Lifshitz, Slyozov and Wagner (LSW) [3] is based on the assumption that in the dilute regime particles interact with each other only via a spatially constant mean-field which leads to a closed

equation for the one-particle number density $f(R, t)$, given by

$$\partial_t f + \partial_R \Big( \frac{1}{R^2} \Big( \frac{R}{\langle R \rangle} - 1 \Big) f \Big) = 0,$$

(1)

$$\langle R \rangle = \frac{\int R f \, dR}{\int f \, dR}.$$

Equation (1) has a one-parameter family of self-similar solutions with compact support. LSW predict in their classical theory that one particular of those profiles, the one with the largest support, characterizes the large-time behavior of all solutions. By now it is however well-known that the long-time behavior of (1) is not universal but depends very sensitively on the data [1, 5], more precisely on the end of the support of the initial data. In order to overcome this weak selection of self-similar asymptotic states we consider higher order effects which have been neglected in the LSW theory and which are due to the finiteness of the volume fraction of particles.

In particular we investigate fluctuations in the particle densities due to screening. Screening, analogous to electrostatic screening, implies that the interaction range of a particle is not infinite, as assumed in the mean-field theory, but finite. A simple scaling argument implies that the expected correction in the equation for the particle number density is of order $\phi^{1/2}$ if $\phi \ll 1$ is the volume fraction of the particles. A theory which proposes a closed equation for the one- and two-particle number densities has been developed in [4] and rederived in mathematically more rigorous way in [2]. However, the theory is based on the assumption that correlations are uniformly small in size space, which is not satisfied for the largest particles in the system. For the largest particles, a boundary layer appears, which is analyzed in [7]. The main part in the analysis is the derivation of a closure relation which allows to express averages over the radii of the two-particle density in terms of the one-particle densities, evaluated at a shift. The precise characterization of this shift allows to use Taylors expansion which leads to leading order to the following second order equation for $f$.

(2)        $$\partial_t f + \partial_R \Big( \frac{1}{R^2} \Big( \frac{R}{\langle R \rangle} - 1 \Big) f \Big) = \phi^{1/2} \partial_R \big( D(R) \partial_R f \big),$$

where $D(R) > 0$ is determined via a complicated integral equation and thus depends nonlocally on $f$. It is shown in [7] by an asymptotic analysis that equation (2) has a unique self-similar solution which is a perturbation of the LSW solution of equation (1) with an exponential tail. The corresponding correction to the growth law of the mean radius is of order $\phi^{1/4}$.

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# Smoluchowski's coagulation equation and Burgers turbulence

## GOVIND MENON

### (joint work with Robert L. Pego)

Smoluchowski's coagulation equation is a fundamental mean-field model of clustering processes. The merging of clusters of mass $x$ and mass $y$ to produce clusters of mass $x + y$ occurs at a mass-action rate modulated by a symmetric rate kernel $K(x, y)$. Formally, the evolution equation for the density $n(t, x)$ of the size distribution reads

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

$$(1) \qquad - \int_0^\infty K(x, y)n(t, x)n(t, y)dy,$$

This equation has been used as a model of clustering in a variety of applications, including the aggregation of colloids, droplet formation in clouds, the analysis of algorithms and random graphs, and the kinetics of polymerization. Many kernels arising in applications are homogeneous, that is, there is $\gamma$ such that $K(\alpha x, \alpha y) = \alpha^\gamma K(x, y)$ for every $\alpha, x, y > 0$. The evolution transports mass from small to large scales, and for homogeneous kernels it is often observed that after suitable rescaling the number density approaches a limiting profile. This is known as *dynamic scaling* in the scientific literature.

Relatively little is known for general homogeneous kernels about the existence of self-similar solutions, their asymptotics, and their domains of attraction. However, for a class of solvable kernels $K = 2, x + y$ and $xy$ we obtained a comprehensive description of asymptotic dynamics [3]. A sample result is the following. To be concrete, we focus attention on the kernel $K = x + y$. In this case, there is a one-parameter family of self-similar solutions with profiles $n_\alpha$, $\alpha \in (1, 2]$. $n_2(x)$ decays exponentially as $x \to \infty$, however $n_\alpha(x)$ has algebraic decay (heavy tails) for $\alpha \in (1, 2)$. A necessary and sufficient condition for initial measure-valued data $\nu_0$ (with $\nu_0(dx) = n(0, x)dx$ when $\nu_0$ has a density) to approach self-similar is

$$\int_0^x x^2 \nu_0(dx) \sim x^{2-\alpha} L(x), \quad x \to \infty,$$

where $L$ is a function slowly-varying at infinity in the sense of Karamata. This result was obtained in [2] and should be considered completely analogous to the characterization of domains of attraction in the central limit theorem. This suggests the utility of classical limit theorems in probability as tools to study models of clustering. This viewpoint is developed further in [3].

There is a striking connection between Smoluchowski's coagulation equation with this kernel, and the problem of Burgers turbulence discovered by Bertoin [1]. Burgers approach to turbulence was to study the statistics of shocks in the entropy solution to Burgers equation $u_t + uu_x = 0$ generated by random initial data $u_0$. For example, if $u_0$ is a Brownian motion, then for $t > 0$ the solution consists of a dense set of shocks, and these shocks coalesce as time increase. More generally, for a large class of random initial data (Lévy processes with downward jumps), the process of shock coalescence is decsribed by Smoluchowski's coagulation equation. This allows us to prove necessary and sufficient conditions (that is, characterize the *universality classes*) in this simplified model of turbulence. These results are stated precisely in [4].

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## Tartar's conjecture, localization of quasiconvex hulls and incompatible sets of gradients
### László Székelyhidi Jr.

Let $\Omega \subset \mathbb{R}^2$ be a bounded open set. Our interest lies in compactness properties of sequences of approximate solutions to inclusions of the type

(1)                              $Du(x) \in K$ for almost every $x \in \Omega$

for functions $u : \Omega \to \mathbb{R}^2$, where $K \subset \mathbb{R}^{2 \times 2}$ is a given compact set.

It is well known that for such problems the main obstruction to compactness is due to the possible presence of rapid oscillations in the sequence of gradients $Du_j$. Indeed, if $A, B \in \mathbb{R}^{2 \times 2}$ are any two matrices such that $\operatorname{rank}(A - B) = 1$, then one can construct a sequence of uniformly Lipschitz functions $u_j$ whose gradients oscillate between $A$ and $B$, and no subsequence of $\{Du_j\}$ converges strongly in $L^1(\Omega)$. If $A$ and $B$ are such that $\operatorname{rank}(A - B) = 1$, we say that $A$ and $B$ are *rank-one connected* and in general speak of rank-one connections. Thus a necessary condition for compactness in (1) is that $K$ contains no rank-one connections. In [13] L. Tartar conjectured that in fact this condition should also be sufficient,

although subsequently (see [14]) he produced an example of a set $K$ consisting of four matrices where there are no rank-one connections but compactness fails. Such examples are nowadays called $T_4$ configurations. On the other hand the conjecture was verified by V. Šverák in [11] for *connected* sets $K \subset \mathbb{R}^{2 \times 2}$.

One of our main results in [5] - in joint work with Daniel Faraco - is that the additional condition that $K$ contains no $T_4$ configurations is indeed sufficient for compactness. We remark that there is a very quick algorithm for testing for $T_4$ configurations, see [12].

**Theorem 2** (D. Faraco - L.Sz. '06). *Suppose $K \subset \mathbb{R}^{2 \times 2}$ is a compact set without rank-one connections and $K$ contains no $T_4$ configurations. Then for any uniformly Lipschitz sequence $u_j : \Omega \subset \mathbb{R}^2 \to \mathbb{R}^2$ with $\mathrm{dist}\,(Du_j, K) \to 0$ in $L^1(\Omega)$, the sequence $\{Du_j\}$ is compact in $L^1(\Omega)$.*

Our methods also allow us to prove a structure theorem for the quasiconvex hulls of compact sets of $2 \times 2$ matrices, in the style of the well-known structure theorem for the rank-one convex hull, e.g. [6].

**Theorem 3** (D. Faraco - L.Sz. '06). *If $K \subset \mathbb{R}^{2 \times 2}$ is a compact set and $K^{qc} \subset \bigcup_{i=1}^{n} U_i$ for pairwise disjoint open sets $U_i$, then $K^{qc} \cap U_i = (K \cap U_i)^{qc}$.*

It should be noted, that whereas the usual proofs of the structure theorem for the rank-one convex hull rely on the locality of rank-one convexity, in the case of quasiconvexity locality is not true in general dimension (see [8]), and in particular it is not known in the case of $2 \times 2$ matrices. In fact this issue is related to Morrey's conjecture regarding quasiconvexity and rank-one convexity.

Our approach is based on the notion of *incompatible sets*. Following [2] we call two disjoint compact sets $K_1, K_2 \subset \mathbb{R}^{2 \times 2}$ *homogeneously incompatible* if whenever $u_j : \Omega \subset \mathbb{R}^2 \to \mathbb{R}^2$ is a sequence of uniformly Lipschitz mappings which are affine on the boundary and such that $\mathrm{dist}\,(Du_j, K_1 \cup K_2) \to 0$ in $L^1$, then either $\mathrm{dist}\,(Du_j, K_1) \to 0$ or $\mathrm{dist}\,(Du_j, K_2) \to 0$. Furthermore if the above holds with no restriction on the boundary values of $u_j$, then the sets $K_1, K_2$ are called *incompatible*. Our method to proving Theorems 2 and 3 is to find a decomposition of $K$ into homogeneously incompatible sets. We build on the ideas developed in [12] to arrive at a sufficiently large class of sets which give rise to pairs of homogeneously incompatible sets. Such sets will be given as the *quasiconformal envelope* $\mathcal{E}_\Gamma$ of closed curves $\Gamma \subset \mathbb{R}^{2 \times 2}$. The key point is to realize that the set $\mathcal{E}_\Gamma$ corresponds on the one hand to elliptic equations and on the other hand to families of quasiconformal mappings. More precisely, if $u \in W^{1,2}(\Omega, \mathbb{C})$ satisfies $Du(z) \in \overline{\mathcal{E}_\Gamma}$ for almost every $z \in \Omega$, then $u$ solves a corresponding nonlinear Beltrami equation of the form

$$\partial_{\bar{z}} u = H(z, \partial_z u),$$

whereas when coupled with appropriate boundary conditions $u$ gives rise to a family of quasiconformal mappings parametrized by the curve $\Gamma$ as

$$u^t(z) = u(z) - \Gamma(t)z.$$

The former allows us to use the approach in [1] to construct certain nonlinear operators which act as projectors onto the set $\mathcal{E}_\Gamma$, whereas the latter, an idea which appeared in [3], leads to the required incompatibility result for solutions of the inclusion $Du(z) \in \overline{\mathcal{E}_\Gamma}$. Indeed, our proof of this incompatibility relies heavily on adapting the methods in Section 7 of [3] - where $\Gamma$ is a straight line in the conformal plane - to our nonlinear setting.

In further work joint with Bernd Kirchheim [7] we show that in fact homogeneously incompatible sets in $\mathbb{R}^{2\times2}$ are incompatible (i.e. with no restriction on the boundary values); in other words for compact sets of $2 \times 2$ matrices homogeneous incompatibility and incompatibility turn out to be equivalent. In particular we obtain the following characterization of sets of gradients of Lipschitz mappings:

**Theorem 4** (B. Kirchheim - L.Sz. '06)**.** *Let $u \in Lip(\Omega, \mathbb{R}^2)$. Then $\{Du(x) : x \in \Omega\}^{rc}$ is connected.*

One consequence of this result combined with Theorem 2 is that if $K_1, K_2 \subset \mathbb{R}^{2\times2}$ are disjoint compact sets which are incompatible for laminates, then there exists a quantitative rigidity estimate of the form

$$\min\left(\int_\Omega \text{dist}\,(Du, K_1)^p, \int_\Omega \text{dist}\,(Du, K_2)^p\right) \leq C_{p,\Omega} \int_\Omega \text{dist}\,(Du, K_1 \cup K_2)^p.$$

Here $1 \leq p < \infty$ and $\Omega$ is any connected Lipschitz domain. This estimate, under the assumption that $K_1, K_2$ are incompatible sets, was recently obtained in joint work with Camillo De Lellis in [4].

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## Liquid crystals in polyhedral geometries
JM Robbins
(joint work with A Majumdar and M Zyskin)

### Overview
Motivated by recent prototype bistable liquid crystal displays, we analyse a continuum model of nematic liquid crystals in confined polyhedral geometries. Our interest is in the topology, energetics and regularity properties of equilibrium configurations, with a view towards identifying and investigating topological mechanisms for bistability. Our results are mainly analytical with some numerics. There are a number of open questions.

Results so far include: homotopy classification of continuous $S^2$-valued maps on polyhedra in $\mathbb{R}^3$ subject to tangent boundary conditions; a lower bound for the infimum one-constant (ie, Dirichlet) energy for given homotopy type, expressed in terms of a generalised minimal connection; for a rectangular prism, upper bounds for the infimum energy, with the same dependence on homotopy type as the lower bound; a topological mechanism for the observed bistability in the PABN (post-aligned-bistable-nematic) device developed by Hewlett-Packard.

### Background
*Frank-Oseen model and harmonic maps.* In the Frank-Oseen model [1], the mean local orientation of the rod-like molecules of a nematic liquid crystal is described by a unit-vector field $\mathbf{n}(\mathbf{r})$, with energy density given by

$$K_1(\operatorname{div}\mathbf{n})^2 + K_2(\mathbf{n}\cdot\operatorname{\mathbf{curl}}\mathbf{n})^2 + K_3(\mathbf{n}\times\operatorname{\mathbf{curl}}\mathbf{n})^2 + K_4\operatorname{div}((\mathbf{n}\cdot\nabla)\mathbf{n} - (\operatorname{div}\mathbf{n})\mathbf{n}).$$

The elastic constants, $K_j$, are material-dependent. To simplify the analysis one often employs the one-constant approximation, $K_1 = K_2 = K_3 = 1, K_4 = 0$, which yields the Dirichlet energy density $(\nabla\mathbf{n})^2$. Minimisers of the Dirichlet energy are $S^2$-valued harmonic maps.

The existence and regularity properties of $S^2$-valued harmonic maps on a domain $\Omega \subset \mathbb{R}^3$ with fixed boundary data $\boldsymbol{\nu} : \partial\Omega \to S^2$ have been extensively studied (see, eg, [2, 3]). It turns out that, even if the boundary map is contractible, the minimiser may not be continuous; it may be energetically favourable to have point defects in the interior of $\Omega$. This is a manifestation of the gap phenomenon, where the infimum of the Dirichlet energy over the space of continuous maps $C^0_{\boldsymbol{\nu}}(\Omega, S^2)$ is strictly greater than the infimum over the space of Sobolev maps $H^1_{\boldsymbol{\nu}}(\Omega, S^2)$.

Brezis, Coron and Lieb [4] determined the infimum Dirichlet energy of $S^2$-valued maps with certain prescribed singularities. For example, consider maps on $\mathbb{R}^3$, approaching a constant value at spatial infinity, which are continuous except at $2n$ points, half of which are defects of degree $+1$, the other half defects of degree $-1$ (higher degrees are described by letting the some of the points coincide). A minimal connection is a pairing of positive and negative defects whose length $L$, given by the sum of distances between paired defects, is a minimum over all possible pairings. The infimum Dirichlet energy is then $8\pi L$.

*Bistable displays.*     Conventional liquid crystal display cells (eg, the twisted nematic cell) support a single equilibrium configuration. To sustain an optically contrasting configuration, an external field is required. This field consumes power. A bistable display cell supports two (or more) optically constrasting equilibrium configurations. Power is required only to switch between but not to maintain them. One mechanism for engendering bistability is to produce cells with featured geometries (eg bumps, ridges, holes) [5, 6].

*Tangent boundary conditions.*     A unit-vector field $\mathbf{n}(\mathbf{r})$ on a polyhedron $P$ is said to satisfy tangent boundary conditions, or to be tangent, if, on each face of $P$, $\mathbf{n}$ takes values tangent to that face. Tangent boundary condition model the behaviour of nematics on certain substrates. On the edges of $P$, $\mathbf{n}(\mathbf{r})$ is necessarily parallel to the edges, and therefore discontinuous at the vertices. Let $C_t(P, S^2)$ denote the space of tangent unit-vector fields on $P$ which are continuous away from the vertices.

## Results
*Homotopy classification. Wrapping numbers.* [7, 8]   The wrapping numbers constitute one set of classifying invariants for the homotopy classes of $C_t(P, S^2)$. They are defined as follows. Let $C_a$ denote a surface in $P$ which separates the vertex $a$ from the other vertices. Consider all points (unit vectors) on $S^2$ which are tangent to one of the faces of $P$; these lie on great circles which partition $S^2$ into disjoint open sets, called sectors. Given a sector $\sigma$ and a vertex $a$, the wrapping number $w_{a\sigma}$ is the (integer) degree of a regular value $\mathbf{s} \in \sigma$ of the restricted map $\mathbf{n} : C_a \to \sigma$ (roughly, the number of times the image of $\mathbf{n}(C_a)$ covers $\sigma$, counted with orientation). Not all values of the wrapping numbers can be realised. Continuity implies that, for each sector $\sigma$, $\sum_a w_{a\sigma} = 0$. There are further constraints (more readily expressed in terms of an alternative set of invariants).

*Lower bound for Dirichlet energy.*     [9, 10, 8, 11]     Let $h \subset C_t(P, S^2)$ denote a homotopy class with wrapping numbers $w_{a\sigma}$. Let $E_{\text{inf}}(h)$ denote the infimum Dirichlet energy over $h$. Then

$$E_{\text{inf}}(h) \geq 2 \sum A_\sigma L_\sigma,$$

where $A_\sigma$ is the area of the sector $\sigma$ and $L_\sigma$ is the length of a minimal connection for a set of point defects at the vertices of $P$ with degrees $w_{a\sigma}$ ($\sum_a w_{a\sigma} = 0$ implies $L_\sigma$ is well defined).

*Upper bounds for rectangular prism.* [10, 8, 11]   For $P$ a rectangular prism, $E_{\inf}(h)$ may be bounded from above by

$$E_{\inf}(h) \leq 2C\kappa^3 \sum_\sigma A_\sigma L_\sigma,$$

where $\kappa$ is the largest aspect ratio of the prism, and $C$ is a constant independent of homotopy type and the aspect ratios. For reflection-symmetric topologies, in which the wrapping numbers at vertices related by a reflection differ by a sign, $C\kappa^3$ can be sharpened to $\sqrt{3}\kappa$.

*PABN cell.* [12]   The PABN has a nonconvex polyhedral geometry consisting of a two-dimensional array of vertical rectangular posts mounted beween two horizontal planar substrates. There is a gap between the top of the posts and the upper substrate. Nematic liquid crystal fills the region between the substrates and posts. The device is observed to be bistable. We have identified some simple nematic topologies (with minimal wrapping numbers) and numerically computed local minimisers of the Frank-Oseen energy with these topologies. The topologies and energetics are compatible with the observed optical and switching characteristics.

## Questions

We would like to establish the existence and regularity properties of minimisers of different topologies. Numerics and heuristic arguments indicate that for the simplest topologies minimisers always exist, for others they may exist or not depending on the geometry, whereas for most topologies minimisers do not exist at all. Another current interest is in relaxed energies for these problems. We are also interested in the dynamics of configurations under applied fields.

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## Two-scale modeling for Hamiltonian systems: formal and rigorous results

### ALEXANDER MIELKE

(joint work with Johannes Giannoulis and Michael Herrmann)

We study how Hamiltonian structures reduce from a microscopic lattice model under the transition to a macroscopic continuum model. Thus, we provide tools for constructing effective macroscopic Hamiltonians. In particular, we are interested in the case of modulations of plane waves having a microscopic structure. Embedding the discrete system into a continuum one and using additional microscopic phase variables we are led to a completely equivalent continuous system that has additional first integrals associated with the translationally invariants in space and phase variables. The phase velocity of the microstructure and the group velocity of modulating pulse can then be factored out and suitable scalings lead to a singularly perturbed system. Arguing formally the Hamiltonian converges to a generalized Γ-limit that governs the macroscopic modulation equation. Only for a system without microstructure we are able to make the limit rigorous in showing weak convergence to a nonlinear Klein-Gordon equation.

The derivation of macroscopic equations for discrete models (or continuous models with microstructure) can be seen as a kind of reduction of the infinite dimensional system to a simpler subclass. If we choose well-prepared initial conditions, we hope that the solution will stay in this form and evolve according to a slow evolution with macroscopic effects only. We may interpret this as a kind of (approximate) invariant manifold, and the macroscopic equation describes the evolution on this manifold, the functions $A$ defining kind of coordinates. We refer to [Mie91] for exact reductions of Hamiltonian systems and to [DHM06, GHM06a, Mie06b, GHM06b] for the full details.

### 1. DERIVATION OF NLS VIA HAMILTONIAN TWO-SCALE REDUCTION

As the easiest example we consider the one-dimensional Klein-Gordon chain

$$\ddot{x}_j = x_{j+1} - 2x_j + x_{j-1} - ax_j - bx_j^3, \quad j \in \mathbb{Z}.$$

The sum of the kinetic and potential energy gives the Hamiltonian

$$H(\mathbf{x}, \dot{\mathbf{x}}) = \sum_{j \in \mathbb{Z}} \left( \tfrac{1}{2}\dot{x}_j^2 + \tfrac{1}{2}(x_{j+1}-x_j)^2 + \tfrac{a}{2}x_j^2 + \tfrac{b}{4}x_j^4 \right).$$

We embed the discrete chain on $\mathbb{Z}$ into the cylinder $\Xi = \mathbb{R} \times \mathbb{S}^1$, where $\mathbb{S}^1$ contains the additional microscopic phase variable. The continuous Hamiltonian system is

(1)
$$\partial_t^2 u = \Delta_{(1,0)} u - au + bu^3 \quad \text{with } a > 0, \quad u \in \mathrm{L}^2(\Xi),$$
$$\text{and } \Delta_{(\varepsilon,\delta)} u(\eta, \phi) := u(\eta+\varepsilon, \phi+\delta) - 2u(\eta, \phi) + u(\eta-\varepsilon, \phi-\delta).$$

Introducing $p = \partial_\tau u$ this is a canonical Hamiltonian system with

$$H^{\mathrm{cont}}(u,p) = \int_\Xi \tfrac{1}{2}p^2 + \tfrac{1}{2}\big(\nabla_{(1,0)}u\big)^2 + \tfrac{a}{2}u^2 + \tfrac{b}{4}u^4 \, \mathrm{d}\eta \, \mathrm{d}\phi.$$

This system contains the KG chain exactly, because it decouples completely into an uncountable family of KG chains just displaced by $(\eta, \phi) \in [0,1) \times \mathbb{S}^1$. Moreover, (1) is invariant under translations in the spatial direction $\eta$ as well as in the phase direction $\phi$. This leads to the two first integrals $I^{\mathrm{sp}}(u,p) = \int_\Xi p \, \partial_\eta u \, \mathrm{d}\eta \, \mathrm{d}\phi$ and $I^{\mathrm{ph}}(u,p) = \int_\Xi p \, \partial_\phi u \, \mathrm{d}\eta \, \mathrm{d}\phi$. Using the symmetry transformation

$$(\widetilde{u}, \widetilde{p}) = T_{ct}^{\mathrm{sp}} T_{(\omega-c\theta)t}^{\mathrm{ph}}(u,p), \qquad \widetilde{\mathcal{H}} = \mathcal{H} - cI^{\mathrm{sp}} - (\omega-c\theta)I^{\mathrm{ph}}$$

the associated canonical Hamiltonian system $\mathbf{\Omega}^{\mathrm{can}}(\widetilde{u}_t, \widetilde{p}_t) = \mathrm{D}\widetilde{\mathcal{H}}(\widetilde{u}, \widetilde{p})$ on $\mathrm{L}(\Xi)^2$ is still fully equivalent to a family of uncoupled KG chains.

Introducing a suitable scaling, which anticipates the desired microscopic and macroscopic behavior, will exposes the desired limit. For this we let

$$(\widetilde{u}(\eta,\phi), \widetilde{p}(\eta,\phi)) = (\varepsilon U(\varepsilon\eta, \phi-\theta\eta), \varepsilon P(\varepsilon\eta, \phi-\theta\eta)),$$

which keeps the canonical structure (after moving a factor $\varepsilon$ arising from $\mathrm{d}y = \varepsilon \, \mathrm{d}\eta$ into the time parametrization $\tau = \varepsilon^2 t$). We obtain the new Hamiltonian

$$\mathcal{H}_\varepsilon(U,P) = \int_\Xi \tfrac{1}{2\varepsilon^2}\Big(\big[P - \omega U_\phi - \varepsilon c U_y\big]^2 + \big(\nabla_{(\varepsilon,\theta)}U\big)^2$$
$$+ aU^2 - \big[\omega P U_\phi + \varepsilon c P U_y\big]^2\Big) + \tfrac{b}{4}U^4 \, \mathrm{d}y \, \mathrm{d}\phi,$$

where $\nabla_{(\varepsilon,\theta)}U(y,\phi) = U(y+\varepsilon, \phi+\theta) - U(y,\phi)$. The modulation ansatz now reads

$$(U(y,\phi), P(y,\phi)) = R_\varepsilon(A)(y,\phi) = (\mathrm{Re}\, A(y)\mathrm{e}^{\mathrm{i}\phi}, \omega\, \mathrm{Re}\, A(y)\mathrm{e}^{\mathrm{i}\phi}) + O(\varepsilon),$$

and leads to $\mathcal{H}_\varepsilon(R_\varepsilon(A)) = \mathbb{H}_{\mathrm{nlS}}(A) + O(\varepsilon)$ and $\mathrm{D}R_\varepsilon(A)^* \mathbf{\Omega}^{\mathrm{can}} \mathrm{D}R_\varepsilon(A) = \mathbf{\Omega}^{\mathrm{red}} + O(\varepsilon)$ with

$$\mathbb{H}_{\mathrm{nlS}}(A) = \int_\mathbb{R} \omega\omega''|A_y|^2 + \tfrac{3b}{8}|A|^4 \, \mathrm{d}y \qquad \text{and} \qquad \mathbf{\Omega}^{\mathrm{red}} = 2\mathrm{i}\omega.$$

Thus, the macroscopic limit is the one-dimensional nonlinear Schrödinger equation

$$2\mathrm{i}\omega A_\tau = -2\omega\omega'' A_{yy} + \tfrac{3}{2}b|A|^2 A.$$

A rigorous justification of this micro-macro transition is given in [GM04, GM06].

## 2. A weak convergence result

For static problems there is a rich literature concerning the $\Gamma$-convergence of potential energy functionals of discrete models to continuum models (cf. [FJ00, FT02, BG02, BLM06]). Here we want to summarize some first results for dynamic problems that rely on weak convergence. In [Mie06a] it was shown that linear elastodynamics can be derived from a general linear lattice model. However, this result used exact periodicity and linearity in an essential way. The

abstract approach presented in [Mie06b] has its main advantage in the flexibility, which allows for applications in nonlinear and macroscopically heterogeneous settings.

In particular, it can be applied to polyatomic Klein–Gordon chains, which we also allow to have large-scale variations in the stiffness and masses. The KG chains under consideration are assumed to have a periodicity of $N$ on the microscopic level, may change also on the macroscopic scale $y = \varepsilon j$, and are all bounded from below by a positive constant. The KG chain is then given by the canonical Hamiltonian system on $\ell^2 \times \ell^2$ via

$$(2) \qquad \mathcal{H}_\varepsilon^{\mathrm{discr}}(\mathbf{x}, \mathbf{p}) = \sum_{j \in \mathbb{Z}} \left( \frac{p_j^2}{2m_{[j]}(\varepsilon j)} + \frac{a_{[j]}(\varepsilon j)}{2}(x_{j+1} - x_j)^2 + \frac{\varepsilon^2 b_{[j]}(\varepsilon j)}{2} x_j^2 + \frac{\varepsilon^2 c_{[j]}(\varepsilon j)}{4} x_j^4 \right),$$

where $[j] = j \bmod N$. To derive a suitable continuum model we embed $\ell^2 \times \ell^2$ into $Z_\varepsilon \subset Z = Z_0 = \mathrm{H}^1(\mathbb{R}) \times \mathrm{L}^2(\mathbb{R})$ via

$$(u, v) = E_\varepsilon(\mathbf{x}, \mathbf{p}) \text{ with } (u(\varepsilon j), v(\varepsilon j)) = (x_j, p_j) \text{ for all } j \in \mathbb{Z}$$
$$\text{with } Z_\varepsilon = \big\{ (u, v) \in Z \mid u|_{[\varepsilon j, \varepsilon j + \varepsilon]} \text{ affine}, v|_{(\varepsilon j - \varepsilon/2, \, \varepsilon j + \varepsilon/2)} \text{ constant} \big\}$$

**Theorem** [Mie06b] *Let* $(x^\varepsilon, p^\varepsilon) : [0, T/\varepsilon] \to \ell^2 \times \ell^2$ *be solutions of the canonical Hamiltonian system associated with* $\mathcal{H}_\varepsilon^{\mathrm{discr}}$ *in* (2). *If for* $\tau = 0$ *we have*

$$\begin{pmatrix} I & 0 \\ 0 & M(\cdot, \cdot/\varepsilon) \end{pmatrix} E_\varepsilon \begin{pmatrix} \mathbf{x}^\varepsilon(\tau/\varepsilon) \\ \varepsilon\mathbf{p}^\varepsilon(\tau/\varepsilon) \end{pmatrix} \quad \rightharpoonup \quad \begin{pmatrix} u(\tau) \\ M^*(\cdot)v(\tau) \end{pmatrix} \quad \text{in } Z,$$

*then this convergence holds for all* $\tau \in [0, T]$, *where* $(u, v) : [0, T] \to Z$ *is a solution of the macroscopic wave equation arising from the canonical Hamiltonian system with* $\mathcal{H}_0(u, v) = \int_{\mathbb{R}} \frac{1}{2M^*(y)} v^2 + \frac{A^*(y)}{2}(u')^2 + \frac{B^*(y)}{2} u^2 + \frac{C^*(y)}{4} u^4 \, \mathrm{d}y$, *where* $M^*(y) = \frac{1}{N} \sum_{k=1}^{N} m_k(y)$ *and similarly for* $B^*(y)$ *and* $C^*(y)$, *whereas* $A_*(y) = 1/ \sum_{k=1}^{N} \frac{1}{a_k(y)}$ *is the harmonic mean.*

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# Homogeneization of dislocations dynamics

RÉGIS MONNEAU

In the present work, we are interested in the motion of defects in crystal, called dislocations. These dislocations are curves moving in crystallographic planes of the crystal, when an exterior stress is applied. The motion is given by the normal velocity to the curve, which is proportional to the Peach-Koehler force. This force is the sum of several contributions: the exterior applied stress, the microstress created by other defects in the crystal (like precipitates), and the stress created by the other dislocations lines.

We are interested in computing the effective motion of dislocations densities, for dislocations all contained in a single cristallographic plane with the same Burgers vector.

Mathematically, we use a phase field model to describe the dynamics of several dislocations moving in a periodic medium, and do the homogeneization of these equations. More precisely, we consider the solutions $u^\varepsilon(t, x)$ of

(1)
$$\begin{cases} \partial_t u^\epsilon = \left( c\left(\dfrac{x}{\epsilon}\right) + M^\epsilon\left[\dfrac{u^\epsilon(t, \cdot)}{\epsilon}\right] \right) |\nabla_x u^\epsilon| + h\left(\dfrac{u^\epsilon}{\epsilon}, \nabla_x u^\epsilon\right) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^N, \\[2ex] u^\epsilon(0, x) = u_0(x) & \text{on} \quad \mathbb{R}^N \end{cases}$$

where for the physical application we have $N = 2$, with dislocations in the plane, represented by the level sets $\{u^\varepsilon(t, \cdot) = k\varepsilon\}$ for each integer $k \in \mathbb{Z}$.

Here the function $c(x)$ is Lipschitz-continuous and $\mathbb{Z}^N$-periodic and represents the periodic medium. The function $h(u, p)$ appears in the derivation of the model like a correction term, and is bounded Lipschitz-continuous w.r.t. $(u, p)$, is 1-periodic w.r.t. $u$ and $h(u, p)/|p|$ is bounded.

Finally the operator $M^\varepsilon$ computes the stress created by the interactions with all the dislocations contained in the same plane. Its expression is given by

$$M^\epsilon[U](x) = -U(x) + \int_{\mathbb{R}^N} dz \, J(z)U(x + \epsilon z)$$

where $J \in C^\infty(\mathbb{R}^N)$ is an *even nonnegative* function that satisfies $\int_{\mathbb{R}^N} dz\, J(z) = 1$ and:

there exists $R_0 > 0$ and a function $g > 0$ s.t. for $|z| \geq R_0 : J(z) = \dfrac{1}{|z|^{N+1}}\, g\left(\dfrac{z}{|z|}\right).$

Because we want to pass to the limit as $\varepsilon \to 0$ in this homogeneization problem, we need first to identify a cell problem, which is the following. We consider solutions $w$ of the following equation for any $L \in \mathbb{R}$, $p \in \mathbb{R}^N$

$$(2) \quad \begin{cases} \partial_\tau w = \left(c\,(y) + L + M^1\,[w(\tau, \cdot)]\right) |\nabla_y w| + h\,(w, \nabla_y w) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^N, \\[2mm] w(0, x) = p \cdot y & \text{on} \quad \mathbb{R}^N \end{cases}$$

Then we have the following preliminary result:

**Theorem 1** (Ergodicity). *For any $L \in \mathbb{R}$ and $p \in \mathbb{R}^N$, under the previous assumptions, there exists a unique $\lambda \in \mathbb{R}$ such that the continuous viscosity solution of* (2) *satisfies:*

$$|w(\tau, y) - p \cdot y - \lambda \tau| \leq C \quad on \quad \mathbb{R}^+ \times \mathbb{R}^N$$

*The real number $\lambda$ is denoted by $\overline{H}^0(L, p)$.*

We now can give the precise form of the effective equation:

$$(3) \quad \begin{cases} \partial_t u^0 = \overline{H}^0\left(\mathcal{I}_1[u^0(t, \cdot)], \nabla_x u^0\right) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^N, \\[2mm] u^0(0, x) = u_0(x) & \text{on} \quad \mathbb{R}^N \end{cases}$$

where $\mathcal{I}_1$ is a Lévy operator of order 1 defined for any function $U \in C_b^2(\mathbb{R}^N)$ by:

$$\mathcal{I}_1[U](x) = \int_{|z| \leq 1} (U(x + z) - U(x) - \nabla_x U(x) \cdot z)\, \frac{1}{|z|^{N+1}} g\left(\frac{z}{|z|}\right) dz$$
$$+ \int_{|z| \geq 1} (U(x + z) - U(x))\, \frac{1}{|z|^{N+1}} g\left(\frac{z}{|z|}\right) dz.$$

We can state our main result on this problem (see [1]).

**Theorem 2** (Convergence). *Assume that $u_0 \in W^{2,\infty}(\mathbb{R}^N)$. Then, under the previous assumptions, the bounded continuous viscosity solution $u^\epsilon$ of* (1) *converges locally uniformly in $(t, x)$ towards the bounded viscosity solution $u^0$ of* (3).

Here the Lévy operator $\mathcal{I}_1$ only keeps the memory of the long range behaviour of the operator $M^\epsilon$. On the contrary the effective Hamiltonian $\overline{H}^0$ will keep the memory of the short range behaviour of the interactions.

From the mechanical point of view, this limit model predicts that the plastic strain velocity is given by $\overline{H}^0$ which depends on the dislocations density $\nabla u^0$, and the effective stress $\mathcal{I}_1(u^0)$, here created by the dislocations density itself.

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## Regularity for oscillatory quasilinear systems

CHRISTOF MELCHER

(joint work with Jan Kristensen)

We address the issue of $\varepsilon$-uniform higher regularity in the context of oscillatory monotone operators

$$\mathcal{A}^\varepsilon[v] = -\operatorname{div} a(x/\varepsilon, Dv)$$

acting on vector functions $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}^N$. The associated coefficients $a = a(y, \xi)$ are supposed to be $Y$-periodic in $y$ so that $\varepsilon$ represents the typical length scale of oscillations. For our main result we assume that for some exponent $p \geq 2$ and for some positive numbers $\alpha$, $\beta$, and $M$ the following monotonicity, Lipschitz, and differentiability properties are valid for any $y_1, y_2, y \in Y$ and $\xi_1, \xi_2, \xi \in \mathbb{R}^{n \times N}$:

(H1) $\langle a(y, \xi_1) - a(y, \xi_2), \xi_1 - \xi_2 \rangle \geq \alpha \, |\xi_1 - \xi_2|^2$

(H2) $\left| a(y_1, \xi_1) - a(y_2, \xi_2) \right| \leq \beta \, \left( |y_1 - y_2| + |\xi_1 - \xi_2| \right)$

(H3) $a(y, \xi) = A(y)\, \xi + R(y, \xi)$ where $\left| R(y, \xi) \right| \leq M \, |\xi|^2$.

The tensor $A = A(y)$ is the linearization at $\xi = 0$ which is supposed to be uniformly strictly elliptic. Typical examples for such operators rise from Euler-Lagrange equations for oscillatory variational integrals

$$(1) \qquad \mathcal{F}_\varepsilon(u) = \int_\Omega F(x/\varepsilon, \nabla u(x)) \, dx$$

with smooth integrands $F = F(y, \xi)$ that are $Y$-periodic $y$ and uniformly convex in $\xi$ with quadratic at behavior at zero and with quadratic growth at infinity. For $f \in L^2(\Omega; \mathbb{R}^N)$ we are interested in weak solutions $u_\varepsilon \in W_0^{1,2}(\Omega; \mathbb{R}^N)$ of the quasilinear system

$$(2) \qquad \mathcal{A}^\varepsilon[u_\varepsilon] = \operatorname{div} f \quad \text{in} \ \Omega \quad \text{with} \quad u_\varepsilon|_{\partial\Omega} = 0.$$

It is well-known by the fundamental work by Tartar that as $\varepsilon \to 0$ the corresponding family of weak solutions $(u_\varepsilon)$ is relatively weakly compact in $W^{1,2}$ and cluster at the weak solution $u^*$ of the homogenized problem

$$(3) \qquad \mathcal{A}^*[u] = \operatorname{div} f \quad \text{in} \ \Omega \quad \text{with} \quad u|_{\partial\Omega} = 0.$$

where the $x$-dependence has dropped out, cf. [9, 5]. The coefficients $a^* = a^*(\xi)$ of the homogenized operator $\mathcal{A}^*[u]$ are given in terms of the weak solution $w = w_\xi \in W_{\text{per}}^{1,2}(Y)/\mathbb{R}$ of the auxiliary cell problem $\operatorname{div} a(y, \xi + Dw(y)) = 0$. We have

$$a^*(\xi) = \int_Y a(y, \xi + Dw(y)) \, dy.$$

¿From this representation one reads that the monotonicity and Lipschitz properties (H1) and (H2) persist. The homogenization result for convex variational integrals

(1) phrased in terms of Gamma-convergence is due to Marcellini [7]. Finally the case of quasiconvex intergrands has been carried out independently by Braides [2] and Müller [8]. The corresponding homogenization result, however, differs substantially from the one in the convex case. In fact, the homogenized problem is no longer determined by a single cell problem which leads to microscopic instabilities and the asymptotic failure of strong ellipticity, cf.[6]. This imposes a conceptional obstruction to regularity even in the linear strongly elliptic case, and we stress the fundamental importance of strict monotonicity.

In view of our assumptions the homogenized system (2) exhibits for sufficiently regular $f$ by a fundamental result of Campanato [3] local $L^q$ (with $q > 2$) estimates for second derivatives. Since gradients $\nabla u_\varepsilon$ of approximate solutions oscillate, we cannot expect bounds for second derivatives that hold uniformly as $\varepsilon \to 0$. We show, however, that the corresponding result on the level of the functions $u_\varepsilon$ deduced from Sobolev embedding hold independently of $\varepsilon$. The analysis is motivated by the corresponding uniform estimates for oscillatory linear elliptic systems by Avellaneda and Lin [1]. Our main result is the following:

*Theorem.* If $n \le 4$ and $f \in L^q(\Omega; \mathbb{R}^N)$ with $q > n$ then there exists $\gamma > 0$ so that

$$u_\varepsilon \in C^{0,\gamma}_{\text{loc}}(\Omega; \mathbb{R}^N)$$

with local bounds that are independent of $\varepsilon$. In case $\Omega$ is a domain of class $C^{1,1}$

$$\|u_\varepsilon\|_{C^{0,\gamma}(\Omega)} \le c \, \|f\|_{L^q(\Omega)}$$

for some universal constant $c > 0$ that is independent of $\varepsilon$.

In view of the well-known example of an unbounded $H^1$-solution of strictly elliptic linear system with discontinuous coefficients by De Giorgi [4] the assumption of periodicity is essential for the result. But as the prove will show other structural assumptions (like e.g. quasi-periodicity) that lead to a regular limit problem might be imposed instead. On the other hand the result is sharp regarding the dimension even in the absence of $x$-dependence. Indeed, by a construction by Sverak and Yan [10], there is a smooth uniformly convex functional of quadratic growth that exhibits unbounded minimizers in dimension $n = 5$. The theorem implies in connection with homogenization a compactness result:

*Corollary.* Under the above assumptions there is a sequence $\varepsilon_k \to 0$ and a corresponding sequence of continuous weak solutions $(u_k) \subset W^{1,2}_0(\Omega; \mathbb{R}^N)$ that converge uniformly to the solution $u^*$ of the homogenized problem.

The proof of the theorem is based on a blow-up argument that incorporates information certain homogenized problem. Such an approach has first been used in the context of linear homogenization by Avellaneda and Lin [1]. Indeed, only considering locally only the homogeneous case when $f = 0$, the homogenized problem exhibits, according to Campanato [3], a Morrey space estimate for $Du$ with some exponent $\mu^* \in (2, n)$. That implies a Hölder estimate by Morrey's embedding theorem. The main step is to show that the Morrey estimate carries over to a uniform energy improvement estimate for the finite $\varepsilon$ problem:

*Proposition* 1. For $\mu \in (0, \mu^*)$ there are universal constants $\theta = \theta(\mu) \in (0, 1)$ and $\varepsilon(\mu) > 0$ with the following property: If $v \in H^1(B_r(x))$ is a weak solution of $\mathcal{A}^\varepsilon[v] = 0$ in $B_r = B_r(x)$, then

$$\int_{B_{\theta r}} |Dv|^2 \, dx \le \theta^\mu \int_{B_r} |Dv|^2 \, dx \quad \text{for any} \quad 0 < \varepsilon < \varepsilon(\mu).$$

For some $\lambda > 0$ to be determined, we distinguish the regimes of small radii $r \le \lambda \varepsilon$ and large radii $r \ge \lambda \varepsilon$, respectively. After rescaling the first regime is standard, whereas for the second regime homogenization results for several limiting regimes are used. In addition to $\varepsilon$ and in order to account for the nonlinearity a second scaling parameter $\eta$ given by $\eta^2 = r^{-(n+1)} \int_{B_r} |Dv|^2 \, dx$ that is related to local energy averages comes into play. Accordingly we consider double indexed families

$$\mathcal{A}^\varepsilon_\eta[v] = -\operatorname{div} a_\eta(x/\varepsilon, Dv) \quad \text{where} \quad a_\eta(y, \xi) = a(y, \eta\,\xi)/\eta$$

that satisfy certain rescaled monotonicity and Lipschitz properties uniformly in $\eta > 0$ and exhibit in view of Gehring's lemma higher integrability properties that hold uniformly in $\varepsilon$ and $\eta$. In a crucial step of independent interest we show that asymptotic limits can be taken at once and exhibit Morrey space regularity:

*Proposition* 2. Suppose that $\mathcal{A}^{\varepsilon_k}_{\eta_k}[v_k] = 0$ in $B$ while $\varepsilon_k \to 0$, $\eta_k \to 0$, and $v_k \rightharpoonup v$ weakly in $W^{1,2}(B; \mathbb{R}^N)$. Then $v$ is a weak solution of the homogenized (strictly elliptic) linear problem $\mathcal{L}^* v = 0$. Under the same assumptions but with $\eta_k \to \infty$ there exists a homogenized operator at infinity $\mathcal{A}^*_\infty$ that satisfies (H1) and (H2) and a subsequence so that $v$ is a weak solution of $\mathcal{A}^*_\infty[v] = 0$.

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# Analysis of the (static) Quasicontinuum Method
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(joint work with Endre Süli)

For the numerical simulation of microscopic material behaviour such as crack-tip studies, nano-indentation, dislocation motion, etc., atomistic models are often employed. However, even on the lattice scale, they are prohibitively expensive and, in fact, inefficient. Even in the presence of defects, the bulk of the material will deform elastically and smoothly. It is therefore advantageous to couple the atomistic simulation of a defect with a continuum or continuum-like model away from it. One of the simplest and most popular examples is the quasicontinuum (QC) method originally developed by Ortiz, Phillips and Tadmor in [7] and subsequently improved by many other authors; see [6] for a recent survey article. The basic idea of the QC method is to triangulate an atomistic body as in a finite element method and to allow only piecewise affine deformations in the computation, thus considerably reducing the number of degrees of freedom. By taking every atom near a defect to be a node of the triangulation, one obtains a continuum description of the elastic deformation while retaining a full atomistic description of the defect. In this talk, an overview of the analysis of the QC method to date is given and some recent results are shown.

Despite its growing popularity in the engineering community, the mathematical and numerical analysis of the QC method is still in its infancy. The first noteworthy analytical effort was by Lin [4] who considers the QC approximation of the ground state of a one-dimensional Lennard–Jones model without applied forces. E and Ming [3, 2] analyze the QC method in the context of the heterogeneous multi-scale method, which requires the assumption that a nearby smooth, elastic continuum solution is available. In [5], Lin analyzes the QC method for purely elastic deformation in two dimensions without using such an assumption, but making instead a strong hypothesis (Assumptions 1. and 2. in [5]) on the exact solution of the atomistic model as well as on its QC approximation. Essentially, it is assumed that an exact as well as a QC solution exist and that both lie in a region where the atomistic energy is convex. For lattice domains resembling smooth or convex sets this assumption seems intuitively reasonable but would be difficult to verify rigorously. For lattice domains with 'sharp', 're-entrant' boundary sections or defects we should not expect it to hold. Finally, we would like to mention the work of Legoll et al. [1] where a multi-scale method similar to the QC method is analyzed, however only nearest-neighbour interactions in one dimension are considered which makes it possible to compute the exact solutions analytically. In our own a-priori analysis [8], while still restricted to one-dimensional problems, we make no additional simplifying assumptions. The a posteriori error analysis of the QC method is completely open.

Fix $N \in \mathbb{N}$ and let $\varepsilon = 1/N$. A normalized version of a simple, one-dimensional model is

$$(1) \qquad E(y) = \sum_{i=1}^{N} \sum_{j=0}^{i-1} \varepsilon J\big(\varepsilon^{-1}(y_i - y_j)\big) - \sum_{i=1}^{N} \varepsilon f_i y_i, \qquad y \in \mathbb{R}^{N+1}.$$

For an affine subspace $\mathcal{A}$ with corresponding linear subspace $\mathcal{A}_0$, a full atomistic solution is a deformation $y \in \mathcal{A}$ such that $E'(y; \varphi) = 0$ for all $\varphi \in \mathcal{A}_0$. A Galerkin approximation is given by taking a low-dimensional subspace of $\mathcal{A}$ and $\mathcal{A}_0$ respectively. The QC method is obtained when those approximation spaces are constructed by a finite element interpolation. For the simple model problem (1) an overview of techniques and results for the a priori and a posteriori error analysis is given.

Often, in nonlinear approximation error analysis, it is assumed that an exact solution is smooth and 'stable', and that a numerical solution is 'sufficiently close'. In the case of the QC method, it can be shown that a sufficient (and to some extent even necessary) notion of 'closeness' is a bound on the error in a discrete $W^{1,\infty}$-norm. Using these assumptions it is straightforward to derive a priori and a posteriori error estimates, even for models as complex as the QC method. In this case, the analysis is furthermore not restricted to one dimension. Thus, the two theoretically most important questions in the analysis of the QC method are:

(1.) *A Priori:* Given an exact, stable solution, under which conditions (for example on the QC mesh) can it be approximated by a QC method?

(2.) *A Posteriori:* Given a QC approximation, does an exact solution of the atomistic model exist which the QC solution approximates in a suitable sense?

At least in one dimension it is possible to answer these questions. In [8, 9] we prove the following results:

(1.) *A Priori:* If $y$ is an exact solution of the atomistic model which satisfies certain stability properties (which we characterize completely) and if the QC mesh is such that the interpolation error is below a certain tolerance, then there exists a QC solution which satisfies a quasi-optimal error estimate.

(2.) *A Posteriori:* If $Y$ is a QC solution contained in a neighbourhood where $E''$ is 'stable' and if its residual is sufficiently small then there exists an exact atomistic solution $y$ and we give an a posteriori error estimate between $Y$ and $y$.

The talk concludes with some numerical examples that demonstrate clearly that our results are both non-trivial and relevant for applications. In particular, we are able to compute some numerical solutions which are very close to an unstable regime of the elastic energy but where we can use the 'a posteriori existence' idea outlined in (2.) to show rigorously that the computed QC solution corresponds to an exact solution of the atomistic problem.

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# Rare events in spatially extended systems

Eric Vanden-Eijnden

Dynamical systems are often subject to random perturbations. Even when these perturbations have small amplitude, they have a profound impact on the dynamics on the appropriate time-scale. For instance, the perturbations result in hoppings between regions around the stable equilibrium points of the deterministic dynamical system which would otherwise be impossible. Such hoppings are responsible for metastable phenomena observed in many systems: regime changes in climate, nucleations events during phase transitions, thermally induced switching in micromagnetism, conformation changes of biomolecules and bistable behaviors in genetic switches are just a few examples among many others.

When the amplitude of the random perturbations is small, Wentzell-Freidlin theory of large deviations provides the right framework to understand their effects on the dynamics [4]. Consider a dynamical system whose evolution is governed by the following stochastic differential equation (SDE):

$$(1) \qquad dX^\epsilon(t) = b(X^\epsilon(t))dt + \sqrt{\epsilon}\,\sigma(X^\epsilon(t))dW(t)$$

where $b : \mathbb{R}^n \mapsto \mathbb{R}^n$, $\sigma : \mathbb{R}^n \mapsto \mathbb{R}^n \times \mathbb{R}^n$ and $W(\cdot)$ is a Wiener process on $\mathbb{R}^n$. Assume that $b$ and $a = \sigma\sigma^T$ are bounded and uniformly continuous and $a$ is such that there exists $\mu > 0$ such that for all $x, c \in \mathbb{R}^n$, $\sum_{i,j=1}^n a_{ij}(x)c_i c_j \geq \mu \sum_{i=1}^n c_i^2$. Then, (1) admits a large deviation principle with the following action functional

$$(2) \qquad S_T(\phi) = \frac{1}{2}\int_0^T |\sigma^{-1}(\phi)(\dot{\phi} - b(\phi))|^2 dt, \qquad \phi(\cdot) \in C_{[0,T]}$$

if the integral converges and $S_T(\phi) = +\infty$ otherwise (here $|\cdot|^2$ is the Euclidean norm and $C_{[0,T]}$ denotes the space of absolutely continuous functions mapping $[0, T]$ into $\mathbb{R}^n$).

The action functional (2) gives a rough estimate of the probability that the trajectory $X^\epsilon(t)$, $t \in [0, T]$, $T < \infty$ of the random dynamical system lies in a small neighborhood around a given path $\phi(t)$, $t \in [0, T]$: for any $\delta > 0$,

$$(3) \qquad \mathbb{P}_x\Big\{ \sup_{0 \le t \le T} |X^\epsilon(t) - \phi(t)| \le \delta \Big\} \asymp \exp\left( -\epsilon^{-1} S_T(\phi) \right)$$

where we denote $f(\epsilon) \asymp g(\epsilon)$ if $\log f(\epsilon)/\log g(\epsilon) \to 1$ as $\epsilon \to 0$, $\mathbb{P}_x$ is the probability conditional on $X^\epsilon(0) = x$ and we assumed that $\phi(0) = x$. The estimate (3) implies that the probability or expectation of various events can be evaluated by constrained minimization. For instance, if $B$ is a Borel subset of $\mathbb{R}^n$,

$$(4) \qquad \mathbb{P}_x\left\{ X^\epsilon(T) \in B \right\} \asymp \exp\left( -\epsilon^{-1} \inf_\phi S_T(\phi) \right)$$

where the infimum is taken over all paths $\phi(\cdot)$ such that $\phi(0) = x$ and $\phi(T) \in B$. The minimizer of $S_T(\phi)$ in (4) is also the path of maximum likelihood by which the process $X^\epsilon(\cdot)$ reaches $B$ from $x$.

Large deviations theory also gives estimates on long time intervals $[0, T(\epsilon)]$, with $T(\epsilon) \asymp \exp(\epsilon^{-1} C)$ and $C > 0$. In this context, the relevant object is the quasipotential

$$(5) \qquad V(x, y) = \inf\{S_T(\phi) : \phi(0) = x, \phi(T) = y\}$$

where the infimum is taken over both $\phi(\cdot)$ and $T$. For instance, if the deterministic system associated with (1), that is,

$$(6) \qquad \dot{X}(t) = b(X(t)),$$

possesses exactly two stable equilibrium points, $x_1$ and $x_2$, the basin of attraction of which is a complete partition of $\mathbb{R}^n$, then on large time intervals the dynamics can be reduced to that of a continuous-time Markov chain on the state-space $S = \{x_1, x_2\}$ with rates

$$(7) \qquad k_{1,2} \asymp \exp\left( -\epsilon^{-1} V(x_1, x_2) \right), \qquad k_{2,1} \asymp \exp\left( -\epsilon^{-1} V(x_2, x_1) \right).$$

Similar reductions are possible when (6) possesses more than two stable equilibrium points or even other stable equilibrium structures such as limit cycles, etc. The quasipotential $V(x, y)$ is also the key object to characterize the equilibrium distribution of the process in the limit as $\epsilon \to 0$.

The theory above is well-known and can be extended to situations where (1) is replaced by a stochastic partial differential equation (SPDE) defining a stochastic process $X^\epsilon(\cdot)$ defined on some suitable Hilbert space $H$ [1]. Essentially, this amounts to redefining the Euclidean norm in (2) and (3) by their suitable equivalent in $H$. Our main focus in this talk is the concrete application of the theory to several SPDEs for which the large deviation principle above is known to be valid, and the calculation of the minimizer of the quasipotential (5) when $x$ and $y$ are local equilibrium points for (6). Often this calculation has to be done

numerically, and this requires to rephrase the definition (5) of the quasipotential $V(x,y)$. Indeed, (5) leads to the difficulty that the minimizer of the functional is non-attainable in general because the infimum is only achieved when $T \to \infty$.

To get around this difficulty, instead of formulating the problem in term of paths $\phi(\cdot)$ parametrized by time, we re-formulate the large deviations minimization problem in terms of curves, $\Gamma = \{\varphi(\alpha) : \alpha \in [0,1]\}$ where $\varphi : [0,1] \mapsto \mathbb{R}^n$ (more generally: $\varphi : [0,1] \mapsto H$) parametrizes the curve $\Gamma$ and we are free to impose any constraint on this parametrization like, e.g., that the curve by parametrized by normalized arclength, $|\varphi'| = cst$ (here and below the prime denotes derivative with respect to $\alpha$). Our main result in this direction is that the quasipotential (5) can be expressed as

$$
\begin{aligned}
V(x,y) &= \inf_\varphi \int_0^1 \left( |\varphi'|_a |b(\varphi)|_a - \langle \varphi', b(\varphi) \rangle_a \right) d\alpha \\
&= 2 \inf_\varphi \int_0^1 |\varphi'|_a |b(\varphi)|_a \sin^2 \tfrac{1}{2}\eta \, d\alpha
\end{aligned}
$$
(8)

where, for any $u, v \in \mathbb{R}^n$, $\langle u, v \rangle_a = \langle u, a^{-1}(\varphi)v \rangle$ is the inner product associated with the diffusion tensor $a$ in (1), $|u|_a^2 = \langle u, u \rangle_a$ is the associated norm and $\eta(\alpha)$ is the angle between the curve $\Gamma$ and the drift vector $b(\cdot)$ at point $\varphi(\alpha)$ (and again, all these must be properly redefined in the infinite dimensional context). Notice that (8) is parametrization free, i.e. it is left invariant under reparametrization of $\varphi(\cdot)$, so we are free to add a constraint on this curve, like e.g. that $|\varphi'| = cst$.

In contrast with (5), the minimizer of (8) over all $\varphi$ is attainable in more general circumstances and this is why (8) is more suitable for computations. The curve $\Gamma_\star$ associated with the minimizer $\varphi_\star$ of (8) also admits the following probabilistic interpretation. The quasipotential $V(x,y)$ can alternatively be defined as [4]

$$
(9) \qquad V(x,y) = -\lim_{T \to \infty} \lim_{\delta \to 0} \lim_{\epsilon \to 0} \epsilon \log \mathbb{P}_x \{ \tau_y^\epsilon(x) \le T \}
$$

where $\tau_y^\epsilon(x)$ is the first entrance time in the ball of radius $\delta$ around $y$

$$
(10) \qquad \tau_y^\epsilon(x) = \inf\{ t : X^\epsilon(t) \in B_\delta(y), X^\epsilon(0) = x \}.
$$

Look at the ensemble of paths before they reach $B_\delta(y)$ for the first time at time $\tau_y^\epsilon(x)$, i.e. the different realizations of $X^\epsilon(\cdot)$ on $t \in [0, \tau_y^\epsilon(x))$, conditional on $\tau_y^\epsilon(x) \le T$. Viewed as functions of $t$, these paths will in general have no limit as $\epsilon, \delta \to 0$ and $T \to \infty$. Yet, their graph in $\mathbb{R}^n$ has a limit and this limit is $\Gamma_\star$: for any $\mu \ge 0$,

$$
(11) \qquad \lim_{T \to \infty} \lim_{\delta \to 0} \lim_{\epsilon \to 0} \mathbb{P}_x \left\{ \rho \Big( \bigcup_{0 \le t < \tau_y^\epsilon(x)} X^\epsilon(t), \Gamma_\star \Big) > \mu : \tau_x^\epsilon(y) \le T \right\} = 0,
$$

where $\rho(\Gamma_1, \Gamma_2) = \sup_{x \in \Gamma_1, y \in \Gamma_2} |x - y|$ is the Fréchet distance between the curves $\Gamma_1$ and $\Gamma_2$. In this sense, $\Gamma_\star$ gives some information on the transition pathways between $x$ and $y$. In special circumstances, e.g. if (6) has exactly two stable equilibrium points, $x_1$ and $x_2$ whose basins of attraction partition $\mathbb{R}^n$ and we look

at $V(x_1, x_2)$, the condition that $\tau_x^\epsilon(y) \leq T$ may be removed in (4) (in this case it is also unnecessary to take the limit as $T \to \infty$).

Armed with these results, we can design efficient numerical algorithms for the variational problem in (8) by generalizing the techniques introduced in [2, 3]. These were used to find the quasipotential and analyze the pathways between the stable equilibrium points of the following SDEs (the equation below are written as standard PDEs for the sake of clarity but they are really SPDEs):

The *stochastic Allen-Cahn equation*

$$(12) \qquad u_t = \Delta u - V'(u) + \sqrt{\epsilon}\,\eta_\delta(x, t)$$

where $u : (t, x) \in \Omega \times [0, \infty) \mapsto \mathbb{R}$, $\Omega \subset \mathbb{R}^n$, and $\eta_\delta$ is a spatially mollified spatio-temporal white-noise ($\delta \geq 0$ being the characteristic length in the mollifying kernel and it must be strictly positive if $n > 1$). (12) is studied with Dirichlet or periodic boundary conditions in space.

The *Landau-Lifshitz-Gilbert equation*

$$(13) \qquad m_t = -m \times h - \alpha m \times (m \times h) \quad \text{where} \quad h = -DE(m) + \sqrt{\epsilon}\,\eta_\delta(x, t).$$

Here $m : \Omega \mapsto S^2$, $\Omega \subset \mathbb{R}^3$, is the magnetization vector, $\eta_\delta$ is as above and $DE(m)$ is the derivative of the Landau-Lifshitz magnetization energy

$$E(m) = \frac{\eta}{2} \int_\Omega \|\nabla m\|^2 + Q \int_\Omega \phi(m) + \frac{1}{2} \int_{\mathbb{R}^3} |\nabla u|^2$$

where $u$ is the stray field satisfying $\mathrm{div}(-\nabla u + m) = 0$, $\eta > 0$, $Q > 0$ are parameters and $\phi : S^2 \mapsto \mathbb{R}$ is the anisotropy factor. (13) is to be solved with Neumann boundary conditions.

The following system of *reaction-diffusion equations*:

$$(14) \qquad \begin{cases} u_t = u - u^3 - \alpha u v^2 + u_{xx} + \sqrt{\epsilon}\,\eta^u(x, t) \\ v_t = -\mu(1 + u^2)v + v_{xx} + \sqrt{\epsilon}\,\eta^v(x, t) \end{cases}$$

where $u, v : (t, x) \in [0, L] \times [0, \infty) \mapsto \mathbb{R}$, $\alpha > 0$ and $\mu > 0$ are parameters and $\eta^u$, $\eta^v$ are independent spatio-temporal white-noises and we impose either Dirichlet or periodic boundary conditions.

In the talk, we presented various pathways between equilibrium points of the SPDEs above in different parameter regimes. We also discussed some asymptotic results that can be obtained e.g. in the sharp interface limit of the action functional associated with the Allen-Cahn equation in 1 and 2 spatial dimensions.

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### Accelerated Molecular Dynamics Methods
ARTHUR F. VOTER

The molecular dynamics (MD) method is an extremely powerful tool for studying problems in chemistry, biology, physics, and materials science. Starting only with a potential describing the forces between atoms, a system is propagated forward in time using Newton's laws, revealing its true dynamical behavior. A major limitation, however, is that because the integration time step is on the order of femtoseconds, simulations are limited to less than one microsecond. This precludes direct simulation of a vast number of interesting and technologically relevant processes.

For many systems, the long-time dynamical evolution consists of infrequent events; the trajectory wanders in each state for a long time, eventually finding a transition path to a new state. We can exploit this behavior to develop an *accelerated molecular dynamics* approach, in which we let the trajectory find an appropriate way to escape from each state, but trick it into doing so more quickly. The result is that the system passes from one state to the next in a dynamically correct way, providing a long-time, state-to-state trajectory. Interestingly, the transitions the system makes are often very different than we would have expected from our intuition. The following provides a brief description of each of the three AMD methods. A review with some applications can be found in Ref. [1].

**Hyperdynamics:** In the hyperdynamics method[2, 3] we assume there are no correlations between successive crossings of the dividing surfaces separating states; i.e., we assume that transition state theory (TST) is exact. We define a bias potential, $\Delta V_b(\mathbf{R})$, which, when added to the original potential, raises the energy in the potential basin but does not change the energy at the dividing surfaces. A key point is that we must design this bias potential without knowing in advance where the dividing surfaces are. This is difficult, but often can be done[3, 4]. The other formal requirement is that the bias potential must preserve the TST-obeying nature of the dynamics. A dynamical simulation on a surface modified in this way has two desirable properties. First, the escape rate from each state is enhanced because the wells are shallower. Second, the relative rates of escape from each state to the various adjacent states are not affected. Consequently, a trajectory on this surface makes transitions at an accelerated rate, and the sequence of transitions is statistically indistinguishable from the sequence that would be obtained from a long trajectory on the original potential.

In hyperdynamics, time is no longer an independent variable, but is instead estimated statistically as the simulation proceeds. At each integration step during the trajectory, the boosted time clock is advanced by the normal MD time step

($\Delta t_{MD}$) multiplied by the inverse Boltzmann factor for the value of the bias potential at that point in configuration space. For a trajectory that has evolved for $n$ steps, the total boosted time (or hypertime) is thus

$$(1) \qquad t_{\text{hyper}} = \sum_{i}^{n} \exp(\Delta V_b(\mathbf{R}_i)/k_B T),$$

where $\mathbf{R}_i$ is the configuration of the system at trajectory step $i$, $k_B$ is the Boltzmann constant, and $T$ is the temperature. In the course of a simulation, the instantaneous boost factor ($\exp[\Delta V_b(\mathbf{R})/k_B T]$) fluctuates exponentially, but in the long-time limit the boosted time converges on the exact time (with vanishing relative error), even if the system escapes from each state before adequately sampling the bias potential and even if every state of the system is different[2]. The average boost factor depends on the bias potential and the system, but tends to increases exponentially as barriers increase or the temperature is lowered.

**Parallel-Replica Dynamics:** In the parallel-replica dynamics method[5], we exploit the fact that infrequent-event processes are first-order. Assuming that any correlated events during the transition to the present basin have ceased, the probability distribution for the time ($t$) until the next escape is given by

$$(2) \qquad p(t) = k_{tot}\exp(-k_{tot}t),$$

where $k_{tot}$ is the sum of all rate constants for escape from this basin. We now consider $M$ replicas of the entire system running independently on $M$ equivalent processors. The key point is that these $M$ replicas behave like a new physical system with $M$ times as many escape paths and a total escape rate $Mk_{tot}$. If the $M$-replica simulation is followed until the first transition occurs on any of the processors, a relatively simple manipulation[5] shows that the correct escape-time distribution [Eq. 2] is recovered, if the time is defined as that accumulated on all the processors up to the instant that one processor detected a transition. Because this replication does nothing to disrupt the relative probabilities of the available escape paths, a simulation in which this approach is repeated for each new state of the system gives a sequence of states and transition times that are indistinguishable from those of a long trajectory on a single processor.

With this approach, infrequent-event dynamics proceed nearly $M$ times faster than a single-processor trajectory, provided the average time between transitions is much longer than the time required to dephase the trajectories initially and the time to evolve the correlated events on one processor following a transition. If implemented properly, parallel-replica dynamics gives the classically exact dynamical evolution for an infrequent-event system. Moreover, any system exhibiting exponentially distributed transition times can be treated with this method, provided the correlation time is known and all state changes can be detected.

**Temperature Accelerated Dynamics (TAD):** In the TAD method[6], escape from each potential basin is accelerated by running at a higher temperature ($T_{high}$) than the desired temperature ($T_{low}$). From among the transitions occurring rapidly at $T_{high}$, the correct $T_{low}$ transitions are allowed, while all others are prevented, so that the system evolves appropriately from state to state. We use a *basin-constrained* trajectory, in which all basin escapes are detected, and then rejected (i.e., the trajectory is reflected back into the basin) until enough information is accumulated to determine which of these attempted $T_{high}$ transitions would occur first at $T_{low}$. TAD assumes the harmonic approximation[7], in which the rate constant for any mechanism $i$ has an Arrhenius form,

$$(3) \qquad\qquad k_i = \nu_i \exp(-E_i/k_B T),$$

where $\Delta E_i$ is the energy difference between the basin minimum and the saddle point and $\nu_i$ is a temperature-independent preexponential factor that depends on the vibrational spectrum at the minimum and the saddle point. Assuming we can find the saddle point (which in turn gives the barrier height $\Delta E_i$) for each of the attempted transitions out of the basin, a simple result emerges: each escape time at $T_{high}$ maps exactly onto a time at $T_{low}$, given by $t_{low} = t_{high} \exp[\Delta E_i (1/k_B T_{low} - 1/k_B T_{high})]$. This is a consequence of the properties of the escape-time distribution for a first-order process [Eq. 2] combined with the simple form in Eq. 3. We thus have a way to determine the ordering of transitions at $T_{low}$. The only remaining issue is knowing when to stop running the $T_{high}$ trajectory. With the additional assumption that all pre-exponentials in the system are greater than some lower bound $\nu_{min}$, this stop time is

$$(4) \qquad\qquad t_{stop} = \frac{1}{\nu_{min}^f} \left[ t_{low}^{short} \nu_{min}^f \right]^{T_{low}/T_{high}},$$

where $t_{low}^{short}$ is the shortest transition time at $T_{low}$, $f$ is the desired confidence (e.g., 0.99) that no later transition would replace the shortest-time transition at $T_{low}$, and $\nu_{min}^f$ is a confidence-modified minimum preexponential factor [$\nu_{min}^f = \nu_{min}/ln(1/(1-f))$]. Once $t_{stop}$ is reached, the transition corresponding to the shortest time is selected, the system is moved to that basin, and the simulation clock is advanced by $t_{low}^{short}$. This TAD procedure is then repeated in the new state.

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## Mechanical interfaces and ionic transport

### Ekhard Salje

The talk focussed on the aspect of thick ferroelastic interfaces in non-metallic materials. It was argued that the thickness of interfaces (twin boundaries) is some nanometres which is sufficient to concentrate ionic transport in these regions (as compared with the bulk of the materials). Experimental evidence was shown for transport of Na and O in WO3 and early melting is a number of examples. As twinboundaries always percolate it means that transport always extends over large distances limited only by the size of the crystal. The case of termination of percolation by the rotation of twin boundaries (i.e. chemical turnstiles) and the formation of needle domains out of two domain boundaries with opposite sign was discussed in detail. The detection of defects of interfaces is not trivial because the concentrations are generally very low. Direct measurements of transport, electrical conductivity etc is one good method. Another is the measurement of the activation energy of the movement of the domain wall. The latter method became possible because it is now understood that lattice pinning (Peierls effect) is irrelevant for thick domain walls so that all pinning is essentially attributed to extrinsic defects. Examples of ferroelastic LaAlO3 were discussed. It was then argued that radiation damage in zircon can be analysed in a similar fashion for leaching and transport of volatile species. The mechanism of radiation damage by radiation cascades was demonstrated leading to amorphized inclusions with a complex internal structure The elastic response of the system shows that the bulk modulus and the shear modulus of zircon soften by ca. 50.

## Domain Evolution in Magnetostrictive Thin Films

### Eckhard Quandt

Different methods (magneto-optic Kerr effect (MOKE) [1], interference contrast colloid technique (ICC) [2], magneto-optic indicator film technique (MOIF) [3] and magnetic force microscopy (MFM) [4]) were used to image the magnetic domain structures in different positive magnetostrictive multilayer and single layer materials as either stress and/or magnetic field was applied. These observations showed that the magnetization vectors rotated under application of an applied perpendicular tensile stress, and recovered upon removal of that stress. The simplest approach to describe the magnetization reversal is to model the total energy

including the effective magnetic anisotropy $K_{k,eff} = K_k + \frac{3}{2}\lambda_s\sigma$ with $K_k$ the magnetic anisotropy constant $\lambda_s$ the saturation magnetostriction and $\sigma$ the applied mechanical stress. In materials with low magnetic anisotropy the development of multiple small-angle domain structure was observed, which formation are due to magnetoelastic energy contributions. Even though the domains developing with stress have general features in common, the resulting domain differ strongly depending on the history of stress. The served domain structures were discussed in view of application as micro-actuators and strain sensor using the magnetostrictive either as a core and a microinductor or as a free layer in tunnel magnetostrictive structures. Special emphasis was led on a reduction of coercivity and on reversibility which is essential for application of these materials. Furthermore, using the ICC method the nature of the domain walls in exchange coupled magnetostrictive multilayers, which are attractive as actuators [5] or sensors [6] were investigated. It was shown that due to magnetostrictive coupling between the stray fields of the domain walls the formation of Niel wall / quasi-Niel wall combinations was favoured.

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## Screening effects in molecules and the linear scaling of energy with volume for a quantum mechanical crystal

Gero Friesecke

(joint work with Stéphane Capet)

We introduce and analyse a simplified model for electrons in molecules [FC06] which allows novel insight into the basic phenomenon of screening. In particular our analysis leads to a simple proof of the Dyson-Lenard theorem in quantum mechanics, in the case where the interatomic distances are bounded away from zero.

## 1. Screening

By screening one means the remarkable tendency of electrons to usually group themselves around the atomic nuclei in such a way so as to cancel much of the long range $\sim 1/R$ Coulomb potential exerted by the nuclei and make the net potential exerted by the atoms short-range.

Screening is usually tacitly assumed in molecular mechanics, molecular dynamics, statistical mechanics, and continuum mechanics. One starts from the outset from short-range atomistic forces respectively short-range continuum forces (i.e. stresses alias surface forces).

Large-scale failure of screening (which is not observed in nature) would lead to spectacular breakdown of these models, e.g. bare Coulomb interactions violate the linear scaling of energy $E$ with volume $V$ for a quantum mechanical crystal. To see this, place bare atomic nuclei on the integer lattice points in a 3D cube of sidelength $L$, $\{R_1, ..., R_M\} = \mathbb{Z}^3 \cap [0, L]^3$ and evaluate their interaction energy asymptotically in the limit of large $L$:

$$E \sim \sum_{\substack{R_\alpha, R_\beta \in \mathbb{Z}^3 \\ |R_\alpha|, |R_\beta| \leq L}} \frac{1}{|R_\alpha - R_\beta|} \sim \iint_{|x|, |y| \leq L} \frac{1}{|x-y|} d(x-y) d(x+y)$$

$$\sim L^3 \cdot L^2 \sim V^{5/3},$$

i.e. the energy per atom tends to infinity as the system gets large (in a finite system of $M = 10^{23}$ atoms it is already too large by a factor of about $10^{17}$).

The above example is unstable, but small-scale failure of screening is common in nature, and yields important $O(1)$ contributions to the energy per atom. Examples include ionic crystals like NaCl, molecules with low permanent multipole moment like $H_2O$, intermediate states during chemical reactions, and single atoms in the core region.

## 2. Rigorous results related to screening

There are no mathematical results which directly explain and quantify screening from quantum mechanics.[1]

This lies at the heart of the absence of mathematical results on quantum $\rightarrow$ continuum scale-bridging.

As an important open problem we mention the bulk (or "thermodynamic") limit problem for a quantum mechanical crystal: Does the ground state energy per unit volume of a large finite crystal converge as the size tends to infinity, and can the limit energy be computed by solving a simpler (e.g. "unit cell") problem? See Lieb and Simon (1977) and Catto, LeBris and Lions (1998) for a resolution for simplified (convex) models and Fefferman (1985) for a treatment of a model system of spinless hydrogen atoms confined by a rigid wall assumption and coupled to an electron "reservoir".

---

[1] An exception is provided by the $R^{-6}$ law for the interaction of isolated, zero angular momenmtum atoms in the "Van der Waals" regime of large separation $R$, see Friesecke and Gardner (2006) for a rigorous account.

However, the fact that the QM ground state energy per unit volume stays *bounded* for a large neutral system has been proved rigorously. This is the content of the celebrated

**Dyson-Lenard theorem** [DL67, LD68] *Given $Z_{max} > 0$, $\gamma > 0$ there exists a constant $c(Z_{max}, \gamma)$ such that for any number $M \in \mathbb{N}$ of atomic nuclei, any number $N \in \mathbb{N}$ of electrons, any nuclear charges $Z_1, .., Z_M \in [0, Z_{max}]$, and any nuclear positions $R_1, .., R_M \in \mathbb{R}^3$ satisfying $\min_{\alpha \neq \beta} |R_\alpha - R_\beta| \geq \gamma$, the corresponding quantum mechanical ground state energy (as defined below) satisfies*

$$E^{QM} \geq -c(M + N).$$

In fact Dyson and Lenard proved the stronger result that $c$ can be chosen independently of $\gamma$.

Note that no regularity (crystalline or other) is required of the nuclei. In particular the result is relevant not just for low-energy configurations of the atomic nuclei, but also for finite temperature considerations.

In the remainder of this note we sketch the simple proof of [FC06] of this fundamental result. The main idea is a successive model reduction quantum –> classical –> continuum and an exact quantification of screening in the continuum model.

This strategy is partially inspired by the work of Lieb and Thirring (1975) who gave a simplified proof via passage to the (semiclassical) Thomas-Fermi model. The advantage of passing instead to the (purely electrostatic) continuum model below is that unlike the TF model, it can be solved explicitly for arbitrary molecules.

## 3. Quantum, classical, and continuum model

Consider a general molecule with $M$ atomic nuclei with charges $Z_1, .., Z_M > 0$ and (clamped) positions $R_1, .., R_M \in \mathbb{R}^3$, and $N$ electrons of charge $-1$.

**Quantum mechanical (non-relativistic, Born-Oppenheimer) energy**

$$E^{QM} = \inf_\Psi \langle \Psi, H\Psi \rangle + V^{nuc},$$

where

$$H = \sum_{i=1}^{N} \left( -\frac{1}{2}\Delta_{x_i} + v(x_i) \right) + \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|},$$

$$v(x) = \sum_{\alpha=1}^{M} \frac{-Z_\alpha}{|x - R_\alpha|}, \qquad V^{nuc} = \sum_{1 \leq \alpha < \beta \leq M} \frac{Z_\alpha Z_\beta}{|R_\alpha - R_\beta|},$$

the $x_i \in \mathbb{R}^3$ are electronic coordinates, the infimum is taken over the usual set of square-integrable, normalized, antisymmetric $N$-electron wavefunctions $\Psi : (\mathbb{R}^3 \times \mathbb{Z}_2)^N \to \mathbb{C}$ with finite kinetic energy, and $\langle \cdot, \cdot \rangle$ denotes the $L^2$ inner product.

**Classical energy**

$$E^{class} = \inf_{(x_1,..,x_N)\in(\mathbb{R}^3\setminus\Omega)^N} V^{class}(x_1,..,x_N) + V^{nuc},$$

$$V^{class}(x_1,..,x_N) = \sum_{i=1}^{N} v(x_i) + \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|}$$

where $\Omega$ is a set of "hard cores" $\cup_{\alpha=1}^{M} B_d(R_\alpha)$ and $B_d$ denotes an open ball of radius $d$. The hard core radius $d > 0$ may be viewed as a classical analogon of $\hbar$. More precisely, the classical energy arises from the quantum energy by replacing the one-body operator $-\frac{1}{2}\Delta_{x_i} + v(x_i)$ by the effective potential $v_{eff}(x_i) := v(x_i)$ when $|x_i - R_\alpha| \geq d$ for all $i$ and all $\alpha$, $+\infty$ otherwise.

**Continuum energy**

$$E^{cont} = \inf_{\mu} I(\mu) + V^{nuc},$$

$$I(\mu) = -\int_{\mathbb{R}^3\setminus\Omega} \sum_{\alpha=1}^{M} \frac{Z_\alpha}{|x - R_\alpha|} d\mu(x) + \frac{1}{2}\int\int_{(\mathbb{R}^3\setminus\Omega)^2} \frac{1}{|x - y|} d\mu(x)d\mu(y),$$

where the infimum is taken over all nonnegative Radon measures $\mu$ on $\mathbb{R}^3\setminus\Omega$ with $\int d\mu \leq N$. (We remark in passing that in a suitable high charge limit at fixed $M$, the continuum functional $I$ is in fact the Gamma-limit of $V^{class}$ [FC06].)

## 4. Comparison estimates and exact continuum minimizer

The Dyson-Lenard theorem follows from three simple lemmas. We take $d = \frac{1}{4}\min_{\alpha\neq\beta}|R_\alpha - R_\beta|$. $c_1$, $c_2$, $c_2$, denote simple explicit constants independent of $M$, $N$, and the $R_\alpha$.

**Lemma 1** $E^{QM} \geq E^{class} - c_1 M$

**Lemma 2** $E^{class} \geq E^{cont} - c_2 N$

**Lemma 3** $E^{cont} \geq -c_3 M$.

Roughly, Lemma 1 holds because the quantum -> classical passage is only a modification of $M$ "one-body" terms (namely introduction of $M$ hard cores, each of which is expected to contain not more than a fixed number of electrons) and Lemma 2 holds because the classical $->$ continuum passage is only a change of $N$ "self-interaction" terms (absent in $E^{class}$ but present in $E^{cont}$). The technical implementation of these observations relies on the Lieb-Thirring inequality respectively Newton's theorem in electrostatics.

The key point, quantifying cancellations between $O(M^2)$ long-range interaction terms, is done in Lemma 3. The proof is so simple that we can include it here. First, replace the delta functions generating the potential $v$ of the nuclei by spherical charge distributions, i.e. introduce

$$\rho := \sum_{\alpha=1}^{M} Z_\alpha \frac{H^2\big|_{S_\alpha}}{4\pi d^2},$$

where $S_\alpha$ denotes the sphere of radius $d$ around $R_\alpha$ and $H^2$ denotes Hausdorff measure (i.e., the usual area element) on the sphere. By Newton's theorem that the electrostatic potential exerted by a radial charge distribution onto a point outside it is the same as that exerted by the same amount of charge placed at the centre of the sphere,

$$v(x) = -\int_{\mathbb{R}^3} \frac{1}{|x-y|} d\rho(y) \quad \text{for all } x \in \mathbb{R}^3 \backslash \Omega.$$

Hence we can rewrite $I(\mu)$ by completing the square,

$$
\begin{aligned}
I(\mu) &= -\int\int_{\mathbb{R}^6} \frac{1}{|x-y|} d\rho(y) d\mu(x) + \frac{1}{2}\int\int_{\mathbb{R}^6} \frac{1}{|x-y|} d\mu(x) d\mu(y) \\
&= \frac{1}{2}\int\int_{\mathbb{R}^6} \frac{1}{|x-y|} d(\rho-\mu)(x) d(\rho-\mu)(y) - \frac{1}{2}\int\int_{\mathbb{R}^6} \frac{1}{|x-y|} d\rho(x) d\rho(y).
\end{aligned}
$$

But the first term is always nonnegative (this is clear for smooth measures, e.g. because $1/|x|$ has a positive Fourier transform, and follows for general measures by approximation [FC06]). In particular, this yields that for neutral molecules or negative ions (i.e. $N \geq \sum_\alpha Z_\alpha$, whence $\mu = \rho$ is an admissible trial function in the variational principle for $E^{cont}$) that the unique minimizer of $I$ is given by $\mu = \rho$ (i.e. in the continuum model, the electrons screen each nucleus exactly) and that – again using Newton's theorem –

$$E^{cont} = -\sum_{\alpha=1}^{M} \frac{Z_\alpha^2}{2d} \geq -c_3 M, \quad c_3 = \frac{Z_{max}^2}{2d}.$$

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## Incompressible plates

GEORG DOLZMANN

(joint work with Sergio Conti)

The rigorous derivation of limiting theories for thin structures by $\Gamma$-convergence methods has been achieved in the past ten years under various assumptions on the scaling of the applied forces, leading to different regimes in the response of the material, see for example LeDret and Raoult [2] for the case of membranes and Friesecke, James, and Müller [3] for plate theories. In this paper we derive the corresponding plate theory for incompressible materials. The proof of our result follows the proof in [3] with suitable changes in order to handle the $p$-growth at infinity and the constraint of incompressibility.

In the following the thin structure is given by $\Omega_h = \omega \times (-h/2, h/2)$ where $\omega$ is an open and bounded domain in $\mathbb{R}^2$ with Lipschitz boundary. In the framework of nonlinear elasticity we consider the total energy given by

$$E_h[u] = \int_{\Omega_h} W(\nabla u)\, \mathrm{d}x.$$

In order to state our $\Gamma$-convergence result, we change the independent variables by $\mathcal{T}_h u(x) = \mathcal{T}_h u(x', x_3) = u(x', hx_3)$ where $h > 0$ and $x' \in \omega$. For $h = 0$ we define $\mathcal{T}_0 u(x') = u(x', 0)$. Thus convergence of a sequence $u_h \in W^{m,p}(\Omega_h)$ to $u \in W^{m,p}(\omega)$ is understood as convergence of $\mathcal{T}_h u_h$ to $\mathcal{T}_0 u$ in $W^{m,p}(\Omega_1)$.

We assume that the free energy density $W$ models an incompressible material,

$$W(F) = \begin{cases} W_0(F) & \text{if } \det F = 1, \\ +\infty & \text{else.} \end{cases}$$

Here $W_0 \in C^0(\mathbb{M}^{3\times 3}; [0, \infty))$, with $W_0(F) = 0$ if and only if $F \in \mathrm{SO}(3)$ and $W_0$ twice continuously differentiable close to $\mathrm{SO}(3)$. Moreover, $W_0$ is frame indifferent, $W_0(RF) = W_0(F)$ for all $R \in \mathrm{SO}(3)$, and $W_0$ satisfies the growth conditions

$$W_0(F) \geq c\, \mathrm{dist}^2\big(F, \mathrm{SO}(3)\big) \text{ close to } \mathrm{SO}(3),$$

$$W_0(F) \geq c|F|^p - \frac{1}{c}, \qquad \text{on } \mathbb{M}^{3\times 3} \text{ with } c > 0, p > 1.$$

We say that a domain $\omega \subset \mathbb{R}^2$ has the approximation property for isometries if all isometries $u \in W^{2,2}(\omega; \mathbb{R}^3)$ can be approximated by smooth isometries in the $W^{2,2}$ norm. This was established by Pakzad [6] for convex domains using a method developed by from Kirchheim [5] to show that $W^{2,2}$ isometries are developable. The same arguments can be extended star-shaped domains. A result for more general domains was recently obtained by Hornung [4]. In the following theorem we denote for $G \in \mathbb{M}^{2\times 2}$ by $\widehat{G} \in \mathbb{M}^{3\times 2}$ the matrix with $\widehat{G}_{ij} = G_{ij}$, $i, j = 1, 2$ and $\widehat{G}_{3i} = 0$, $j = 1, 2$.

**Theorem 5** (Plate theory for incompressible materials). *Suppose that $W$ satisfies the foregoing assumptions and that $\omega$ has the approximation property for isometries. Then the functionals $h^{-3}E_h$ converge to $E_0$ in the sense of $\Gamma$-convergence with respect to the strong $W^{1,p}$-topology where*

$$E_0[u] = \begin{cases} \dfrac{1}{24} \displaystyle\int_\omega Q_2(\mathrm{II}_u)\, \mathrm{d}x' & \text{if } u(x) = u(x') \text{ and } \nabla' u \in W^{1,2}(\omega; \mathrm{O}(2,3)), \\ +\infty & \text{else.} \end{cases}$$

*More precisely, the following assertions hold true:*

*(a) Compactness: If $u_h \in W^{1,p}(\Omega_h; \mathbb{R}^3)$ is a sequence with $E_h[u_h] \leq C < +\infty$ then there exists a subsequence (not relabeled) and a function $u \in W^{2,2}(\omega; \mathbb{R}^3)$ with $\nabla u \in \mathrm{O}(2,3)$ a.e. such that $\mathcal{T}_h u_h \to \mathcal{T}_0 u$ strongly in $W^{1,p}(\Omega_1; \mathbb{R}^3)$.*

*(b) Lower bound: If the sequence $\{u_h\}$ in (a) converges to $u$, then*

$$E_0[u] \leq \liminf_{h \to 0} E_h[u_h].$$

*(c) Upper bound: For all $u \in W^{2,2}(\omega; \mathbb{R}^3)$ with $\nabla u \in \mathrm{O}(2,3)$ a.e. and every sequence $h_j \to 0$ there exist a sequence $u_j \in C^1(\Omega_h; \mathbb{R}^3)$ such that $\mathcal{T}_{h_j} u_j \to \mathcal{T}_0 u$ strongly in $W^{1,p}(\omega; \mathbb{R}^3)$ and*

$$\limsup_{h \to 0} E_h[u_h] \leq E_0[u].$$

*Here $\mathrm{II}_u = (\nabla' u)^T \nabla' b$ is the second fundamental form and $b = \partial_1 u \wedge \partial_2 u$ is the normal vector to the surface parameterized by $u$. Finally,*

$$Q_2(G) = \min_{d \in \mathbb{R}^3, \, \mathrm{Tr}(\widehat{G}|d) = 0} Q_3(\widehat{G}|d) \quad \text{for all } G \in \mathbb{M}^{2 \times 2}$$

*and*

$$Q_3(F) = \nabla^2 W_0(\mathrm{Id})(F, F) \quad \text{for all } F \in \mathbb{M}^{3 \times 3}$$

*is the quadratic form with the moduli of linear elasticity.*

Note that the constraint of incompressibility has been relaxed since changes in the surface area of the cross-section can be accomodated by changes in the thickness of the plate. The case of membrane theory had been treated independently in [8, 7] and in [1].

The proof of Theorem 5 requires an extension of the derivation of the plate theory in [3] under the weaker growth condition at infinity.

**Theorem 6** (Plate theories with $p$-growth at infinity). *Suppose that $W_0$ satisfies the foregoing assumptions. Then the energies*

$$I_h[u] = \frac{1}{h^3} \int_{\Omega_h} W_0(\nabla u) \, \mathrm{d}x$$

*converge in the sense of $\Gamma$-convergence with respect to the strong topology in $W^{1,p}$ to*

$$I_0[u] = \begin{cases} \dfrac{1}{24} \displaystyle\int_\omega Q_2(\mathrm{II}_u) \, \mathrm{d}x' & \text{if } u(x) = u(x') \text{ and } \nabla' u \in W^{1,2}(\omega; \mathrm{O}(2,3)), \\ +\infty & \text{else} \end{cases}$$

*where*

$$Q_2(G) = \min_{d \in \mathbb{R}^3} Q_3(\widehat{G}|d) \quad \text{for all } G \in \mathbb{M}^{2 \times 2}$$

*and $Q_3$ is given as before.*

The proof follows the one in [3] after a suitable truncation of $u_h$. The scaling of the energy as $h^{-3}$ implies that $|\nabla u_h|$ can be large only on a small set.

*Proof of Theorem 5.* The compactness and the lower bound follow from the arguments in [3] with the necessary modifications for $p > 1$ in the proof of Theorem 6. The idea is to approximate $W$ from below with $W^k(F) = W_0(F) + (\det F - 1)^2$.

The upper bound is more subtle since one needs to construct a sequence of functions $u_j$ that satisfy the constraint of incompressibility pointwise. To do this, suppose first that $u$ is smooth; this is possible since $\omega$ has by assumption the approximation property for isometries. Let

$$b(x') = \partial_1 u(x') \wedge \partial_2 u(x'), \quad R(x') = \big(\nabla' u(x'), b(x')\big),$$

and define, following the classical *ansatz*,

$$v(x', x_3) = u(x') + x_3 b(x') + \frac{x_3^2}{2}\, d(x').$$

A short calculation shows that

$$\det \nabla v(x) = 1 + x_3 \operatorname{Tr}\big(R^T(x')(\nabla' b|d)\big) + x_3^2 E(x)$$

where $E$ depends on $u$, $d$ and their derivatives. For a given vector field $d$ with $\operatorname{Tr}\big(R(x')^T(\nabla' b|d)\big) = 0$ the error in the determinant constraint is quadratic in $x_3$. We define a nonlinear change of coordinates by $\Phi(x', x_3) = (x', \phi(x_3))$ and set $w = v \circ \Phi$. The condition $\det \nabla w = 1$ implies an ordinary differential equation for $\phi$ as a function of $x_3$ where the in-plane variables appear only as a parameter. The solution exists for $x_3 \in (0, h_0)$ for some $h_0 > 0$ independent of $x'$. Finally one chooses $d$ in a suitable way to replace $Q_2$ by $Q_3$ on a large set. $\qquad\square$

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## Reversibility and irreversibility
OLIVER PENROSE

In order of increasing detail, some well-known forms of mathematical description for a material object or system of material objects are:

1. The thermodynamic description, which includes the principle that the entropy $S$ of a thermally isolated system never decreases with time :

$$(1) \qquad \text{if} \quad t_1 < t_2 \quad \text{then} \quad S(t_1) \leq S(t_2)$$

2. Macroscopic descriptions, such as the heat equation

$$(2) \qquad \partial e/\partial t = K\nabla^2 T$$

3. Descriptions by kinetic equations such as Boltzmann's equation

$$(3) \qquad \partial f/\partial t + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = I(f)$$

where $I(f)$ is an integral expression representing the effect of collisions on the distribution function $f(\mathbf{v}, \mathbf{x}, t)$ of particle velocities $\mathbf{v}$ at position $\mathbf{x}$.

4. Microscopic representations as a system of particles obeying Newton's equations of motion

$$(4) \qquad m\, d^2\mathbf{x}_i/dt^2 = -\nabla_i V(\mathbf{x}_1, \cdots, \mathbf{x}_N),$$

where $V$ is the potential energy, or Schrödinger's equation for the same system

$$(5) \qquad i\hbar\, \partial\psi/\partial t = \left\{ -(\hbar^2/2m) \sum \nabla_i^2 + V \right\} \psi$$

To verify consistency, one would like to able to derive the less detailed models from the more detailed ones; for example it is easy to deduce (1) from (2). But in trying to derive any of the less detailed models (1,2,3) from microscopic dynamics we encounter a difficulty: the microscopic equations (4) and (5) are 'reversible', i.e. invariant under the time reversal transformation

$$(6) \qquad R: \quad t \to -t, \quad v \to -v, \quad d/dt \to -d/dt, \quad \psi \to \bar{\psi}$$

whereas the less detailed models are 'irreversible', as is the observed behaviour of real physical objects.

This paradox has generated much controversy and some strange remarks, even from scholars of high repute[1]. Mathematically, what the paradox tells us is this: anything that is derived from the microscopic equations (4) or (5) *alone* will have the same time-reversal symmetry as those equations. Since eqns (1,2,3) do not have that symmetry, it follows that they cannot be derived from microscopic mechanics *alone*. The model must contain, in addition, some non-mechanical ingredient[2]. What can this extra non-mechanical ingredient be?

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[1]An example, from p. 375 of Truesdell[7]: ' ... it requires no great mathematician to see that the reversibility theorem and Poincaré's recurrence theorem make irreversible behavior impossible for dynamical systems in the classical sense.'

[2]"There cannot be a rigorous mechanical derivation of the macroscopic equations from the microscopic ones. Some additional information or assumption is indispensable" [5].

The difficulty is that the equations of motion (4) and (5) have too many solutions. Some of these (sometimes called[2, 4] the 'good' solutions) correspond to plausible macroscopic behaviour, but others, the 'bad' solutions, correspond to macroscopic behaviour whose like we never see in the real world — heat flowing from cold to hot, for example. To complete the microscopic description we need some information to pick out the 'good' solutions and reject the 'bad' ones. This information will take the form of a plausible probability assumption.

To formulate the assumption, consider a thought-experiment. A container is separated into two equal parts by a partition. Initially (time $t_0$) the left-hand compartment contains $N$ molecules of gas and the right-hand one is empty. The partition is removed and the gas expands irreversibly into the empty compartment. Soon (time $t_2$) it is distributed approximately evenly between the two compartments. Let us denote the number of molecules in the right-hand compartment by $M$. Initially the value of $M$ is zero, but after the partition is removed we expect it to increase, eventually fluctuating around a mean value of $\frac{1}{2}N$. Correspondingly, the entropy would increase from 0 to a value fluctuating around $k \log\{N!/(\frac{1}{2}N)!^2\} \approx Nk \log 2$, in conformity with eqn (1).

To see how the 'good' solutions were picked out here, let us look at Bricmont's account[2]: 'the overwhelming majority of the microscopic configurations corresponding to the gas in the left half will evolve deterministically so as to induce the observed evolution of $M$. There may of course be some exceptional configurations, for which all the particles stay in the left half. All one is saying is that those configurations are extraordinarily rare, and that we do not expect to see even one of them appearing when we repeat the experiment many times, not even once "in a million years", to put it mildly'.

In the above passage, starting from the fact that a certain special set of configurations (namely those which will evolve deterministically so as to give $M(t_2) = 0$) is in a tiny minority at time $t_0$, it is argued that the set of trajectories evolving from this special set of configurations has a tiny probability. This is tantamount to the following assumption: plausible probabilities for the evolution after time $t_0$ can be obtained from a probability density in the space of dynamical states which at time $t_0$ is uniform over the 'initial' set of dynamical states — those for which $M = 0$. Rather than pick out a specific class of 'good' solutions, the assumption proposes a probability measure under which (for large $N$) 'good' solutions are highly probable. Notice the time-reversal asymmetry: the high-probability solutions are 'good' after time $t_0$, but not necessarily before.

Some of the conclusions that follow from such a probability assumption are:

- For finite systems, the principle of certain entropy increase (1) is replaced by a probabilistic statement[3].
- Irreversibility is qualitative: the more particles in the system, the more irreversibly it behaves (i.e. the more unlikely is the reversed motion). 'Absolute' irreversibility can occur only in the limit of an infinite system.

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[3]This was known to Boltzmann[1] :' My minimum theorem as well as the so-called Second Law of Thermodynamics are only theorems of probability'.

- Any microscopic description using eqn (4) or (5) alone is incomplete: some probability information is needed as well, normally about the initial time[4]. For example, in Lanford's derivation of Boltzmann's equation (3) from microscopic dynamics[3], the particles are assumed to be as uncorrelated as possible at the initial time, and a similar independence assumption is made in Lebowitz and Spohn's derivation of Fick's law for self-diffusion[4].

*Note added after the talk.* A difficulty with the the probability assumption used above is that it refers to a special 'initial' time $t_0$ with no statement of how this time is to be chosen or why it is so special[5]. Moreover, although the probability assumption implies (1) (in a probabilistic sense) in the special case where $t_1 = t_0$, it does not obviously do so for any other value of $t_1$

This difficulty could be avoided by replacing the above probability assumption with the following stronger 'multi-time' assumption: given any time interval $[t_1, t_2]$, if a probability density in the space of dynamical states takes a simple form[6] at time $t_1$, then it induces a probability distribution on trajectories under which the trajectory is very likely to be 'good' on that time interval.

The multi-time probability assumption gives a family of microscopic probability densities for a given material object, each one giving a different mathematical model with its own 'initial' time $t_1$ and its own time interval of validity. These probability densities are not directly observable, and it is not claimed that any of them is the 'true' or 'real' probability density in dynamical space, whatever that means; all that is claimed is that the resulting mathematical models will all give good representations of the observed (probabilistic) behaviour over their resepctive time intervals of validity. That leaves us with a mathematical problem: to show that such a claim is consistent with the equations of mechanics (for a rudimentary discussion of this consistency problem, see [6].).

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[4]Boltzmann again: 'It can never be proved from the equations of motion alone that $H$ [i.e. $-S$] must always decrease. It can only be deduced from the laws of probability, that if the initial state is not specially arranged for a certain purpose, but haphazard [*sic*] governs freely, the probability that $H$ decreases is always greater than that it increases.' [1].

[5]This difficulty may be one of the reasons why some people (including the present author) have tried to trace irreversibility back to the truly special time when the world began. Whatever its merits, that enterprise does not help with the topic of this talk, which is the consistency of different mathematical models for the same material object.

[6]'Simple' needs a proper definition. It could mean, for example, 'uniform over the part of the space compatible with the current macroscopic state'

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# Long-time validity of the gainless homogeneous Boltzmann equation

FLORIAN THEIL

(joint work with Karsten Matthies)

The derivation of the continuum models of mathematical physics from atomistic descriptions is a longstanding and fundamental problem, see problem six in [Hil00]. This article is the first of a series of papers ([MT06a], [MT06b], [MT06c]) where we propose and develop a new method that allows us to derive and justify effective continuum limits as scaling limits of large interacting particle systems. In particular we can confront a fundamental challenge in statistical mechanics: The emergence of irreversible macroscopic behavior generated by deterministic reversible Hamiltonian micro-evolution. For earlier work, which was mostly restricted to short times or linear equations, see [Gal70, Lan75, Spo78, BBS83, Spo91, CIP94] and references therein.

We concentrate on a simplified model where $n$ hard balls with diameter $a > 0$ move along straight lines until they collide and are removed after the collision. The initial positions of the centers of the balls $(u_0(i), v_0(i)) \in \mathbb{T}^d \times \mathbb{R}^d$, $i = 1 \ldots n$ are iid random variables with law $1_{\mathbb{T}^d} \otimes f_0 \in PM(\mathbb{T}^d \times \mathbb{R}^d)$. We send $n$ to infinity and prove rigorously that the weak-* limit of the empirical densities satisfies a simple mean-field theory, *provided* that $f_0 \in M_+(\mathbb{R}^d)$ has finite total mass and kinetic energy

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

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

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

where $\rho(v, \nu) = v + \mathbb{R}\,\nu$.

**Theorem 7.** *(Justification of the gainless Boltzmann equation)*
*Let $f_0 \in PM_+(\mathbb{R}^d), d \geq 2$ be a momentum density that satisfies (1, 2) and let for each $N \in \mathbb{N}$ the initial values $(u_0(i), v_0(i))$, $i = 1 \ldots n$ be such that $\omega = \{(u_0(i), v_0(i)) \mid i = 1 \ldots n\} \subset \mathbb{T}^d \times \mathbb{R}^d$ is a Poisson point process with intensity $N(\mathbf{1}_{\mathbb{T}^d} \otimes f_0)$. Let $u_t(i) = u_0(i) + tv_0(i)$, $v_t(i) = v_0(i)$ and $\beta_t(i) \in \{0, 1\}$ be the*

*indicator function of particles that haven't collided yet. If the diameter of the particles a depends on N such that*

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

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

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

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

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

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

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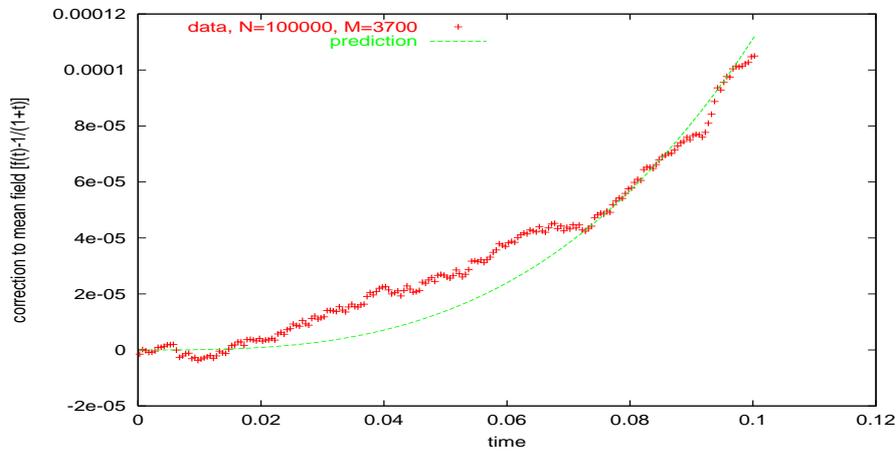


FIGURE 1.    Comparison between the empirical probability of colliding and the mean-field prediction. The dashed line is the cubic parabola $t \mapsto \frac{1}{9}t^3$, the signs '+' mark the difference between the number of non-collided particles at time $t$ divided by $N$ and the mean-field prediction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

**Theorem 8.** *Let $v \in \mathbb{R}^2$ be nonresonant ($\alpha \cdot v \notin \mathbb{Z}$ for all $\alpha \in \mathbb{Z}^d$) such that $|v| = \frac{1}{4}$ and set $f_0 = \frac{1}{2}(\delta(\cdot - v) + \delta(\cdot + v))$. If $\widehat{Q}(t) = \lim_{k,N \to \infty} \mathrm{Prob}(\beta_t(1) = 1)$ denotes the empirical probability that a tagged particle does not collide, then*

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

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

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

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## Kac potentials for elasticity

### STEPHAN LUCKHAUS

Here we try to present a many body Hamiltonian that allows to define elastic strain. The long term goal which at present seems still far away, is a thermodynamic for metastable states for this Hamiltonian.

The Hamiltonian consists actually of 4 parts, one measures the energy of a linear shear, another the deviation of atoms from the sheared lattice position in a localized independent way. This is like a one body Hamiltonian in a mean field of mesoscopic range, which justifies the term Kac potential. Then a term penalizing vacancies is added to avoid crack formation, and a repulsive two body term has to be kept to avoid concentration.

The formula for the Hamiltonian is

$$H\big((x_i)_{i \in I}\big) = \int_\Omega h(x, (x_i)_{i \in I}) dx, \ \{x_i, i \in I\} \subset \Omega$$

where $h$ is given via an auxiliary pointwise minimization problem

$$
\begin{aligned}
h(x,(x_i)_{i\in I}) &= \inf_{A\in Gl(n)^+, z\in\mathbb{Z}^n}\Big[ f_1(x,A,\tau,\zeta,(x_i)_{i\in I}) \\
&\quad + f_2(x,A,\zeta,(x_i)_{i\in I}) + f_3(x,\zeta,(x_i)_{i\in I}) + W(A^{-1})\Big] \\
f_1(x,A,\tau,\zeta,(x_i)_{i\in I}) &= \sum_I W_{per}\Big(A(x_i-x)+\tau\Big)\eta\Big(\frac{x_i-x}{\zeta}\Big) \\
f_2(x,A,\zeta,(x_i)_{i\in I}) &= \zeta^{-n}\Big(\sum_I \eta\Big(\frac{x_i-x}{\zeta}\Big) - \zeta^n det A\Big)^2 \\
f_3(x,(x_i)_{i\in I}) &= \sum_{i\neq j} V(|x_i-x_j|)\eta\Big(\frac{x_i+x_j-2x}{3\zeta}\Big)
\end{aligned}
$$

Here $W_{per}^{-1}(\{0\}) = \mathbb{Z}^n$, $W_{per}(x+z) = W_{per}(x)\forall Z\in\mathbb{Z}^n$, $W_{per}\geq 0$, $D^2 W_{per}(0) > 0$, $\eta$ positive with compact support and $\int\eta = 1$, $V$ positive with compact support, $V(r)\geq\rho > 0$ for $r < \rho$ for some positive $\rho$ and $k$. $W$ the "elastic potential" is invariant under $SO(n)$ and positive.

One is interested in regimes where $\zeta\to\infty$ and $\frac{diam\Omega}{\zeta}\to\infty$.

Just calculating the energy of $x_i$ in the position of a sheared lattice $B\mathbb{Z}^n$, one sees that for these $(x_i)$, (for $n = 2,3$)

$$
\begin{aligned}
h(x,(x_i)_I) &= \inf_{B\in Gl(n,\mathbb{Z})^+} W(B\tilde{B}) + O\Big(\frac{1}{\zeta}\Big) \qquad \text{if } V(\inf(|Bz|, z\in\mathbb{Z}^n) = 0 \\
h(x,(x_i)_I) &\longrightarrow_{\zeta\to\infty}\infty \qquad otherwise.
\end{aligned}
$$

This justifies the name elastic potential for $W$. But it also shows that one should not look at $\Gamma$ convergence or equilibrium measures for this potential.

So what one can do is to characterize low energy states for this Hamiltonian.

The following estimate is helpful in that respect:

**Lemma:** For $K > 0$ arbitrary $\zeta > \zeta_0$ there exists $\varepsilon_\alpha(K), \alpha = 1,2,3$ such that in

$$
\begin{aligned}
\widehat{\Omega}_K &= \big\{(x,A,\tau)| f_\alpha(x,A,\tau,\zeta,(x_i)_{i\in I}) &\leq&\; \varepsilon_\alpha(K), \|A^{-1}\| < K\big\} \\
D^2_{A,\tau} f_1(x,A,\tau,\zeta,(x_i)_{i\in I})\langle(B,\sigma),(B,\sigma)\rangle &\geq&\; c\zeta^n det A\big[|\sigma|^2 + \zeta^2|B|^2\big] \\
D^2_A f_2(x,A,\zeta,(x_i)_{i\in I})\langle B,B\rangle &\geq&\; -c\sqrt{\varepsilon_2}K^2\zeta^n det A|B|^2 \\
|\bigtriangledown_x f_1(x,A,\tau+Ax,\zeta,(x_i)_{i\in I})| &\leq&\; c\zeta^{n-1} \\
|\bigtriangledown_x f_2(x,A,\zeta,(x_i)_{i\in I})| &\leq&\; c\zeta^{n-1}
\end{aligned}
$$

This lemma entails that if $A_x\tau_x$ denote the minimizers of either $f_1(x,A,\tau,...)$ or $W(A^{-1})+f_1(x,A,\tau,...)$ or $W(A^{-1})+f_1(x,A,\tau,...)+f_2(x,A,...)$ these provide a covering of $\Omega_K$ the projection of $\widehat{\Omega}_K$. Moreover $|A_x - \bigtriangledown\tau_x| = O(\frac{1}{\zeta})$ so that there exist local Lagrangian coordinates defined by $\Phi = \tau^{-1}$. Finally one sees that there is a mapping: $\text{Hom}(\Omega_K)\to Gl(n,\mathbb{Z})\times\mathbb{Z}^n$ the group of - approximate-

cover transformations the second of which corresponds to the Burgers vector in the theory of dislocations.

We expect that the theory, depending on the scaling of $\zeta$ versus $diam(\Omega)$ will give a good description of dislocations and graim boundaries.

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## Phase transitions for gradient field models
ROMAN KOTECKÝ
(joint work with Marek Biskup)

Let us consider *gradient fields* $\eta = (\eta_b)$ with $b \in (\mathbb{Z}^d)^*$, $d \geq 2$, the set of all (non-oriented) nearest-neighbour edges in $\mathbb{Z}^d$, and $\eta_b \in \mathbb{R}^m$, $m \geq 1$. (Even though the results in [1] and [2], to which we refer below, are stated and proved for $m = 1$, a generalisation to $m > 1$ is rather straightforward.) Further, let $\mathcal{X} \subset \left(\mathbb{R}^m\right)^{(\mathbb{Z}^d)^*}$ be the linear space defined by imposing the *loop condition* $\eta_{b_1} + \eta_{b_2} = \eta_{b_3} + \eta_{b_4}$ for each plaquette $(b_1, b_2, b_3, b_4)$ in $\mathbb{Z}^d$.

For any even function $V : \mathbb{R} \to \mathbb{R}$ with a sufficient growth at infinity, we consider the set $\text{ext}\,\mathcal{G}(V)$ of all *translation invariant ergodic gradient Gibbs measures* defined by standard DLR equations with respect to the collection of finite volume Gibbs measures $P_{\mathbb{B}}^V(\mathrm{d}\eta_{\mathbb{B}}|\bar{\eta})$. Here, for any finite $\mathbb{B} \subset (\mathbb{Z}^d)^*$ and any $\bar{\eta} \in \mathcal{X}$, we define

$$(1) \qquad P_{\mathbb{B}}^V(\mathrm{d}\eta_{\mathbb{B}}|\bar{\eta}) = \frac{1}{Z_\Lambda(\eta_{\mathbb{B}}|\bar{\eta})} \exp\Big\{-\sum_{b \in \mathbb{B}} V_b(|\eta_b|)\Big\} \nu_{\mathbb{B}}(\mathrm{d}\eta_{\mathbb{B}}|\bar{\eta}),$$

with $\nu_{\mathbb{B}}(\mathrm{d}\eta_{\mathbb{B}}|\bar{\eta})$ denoting an *a priori* uniform measure on the set

$$(2) \qquad \mathcal{X}_{\mathbb{B},\bar{\eta}} = \left\{\eta_{\mathbb{B}} \in \left(\mathbb{R}^m\right)^{\mathbb{B}} \mid \eta_{\mathbb{B}} \vee \bar{\eta}_{\mathbb{B}^c} \in \mathcal{X}\right\}$$

and $Z_\Lambda(\eta_{\mathbb{B}}|\bar{\eta})$ the normalising factor (partition function). A measure $\mu$ on $\left(\mathbb{R}^m\right)^{(\mathbb{Z}^d)^*}$ satisfies DLR equations with respect to the collection $\{P_{\mathbb{B}}^V(\mathrm{d}\eta_{\mathbb{B}}|\bar{\eta})\}$ if

$$(3) \qquad \mu(\cdot \mid \mathcal{F}_{\mathbb{B}^c}) = P_{\mathbb{B}}^V(\cdot|\bar{\eta}), \quad \mu \text{ a.e. } \bar{\eta} \text{ and all finite } \mathbb{B} \subset (\mathbb{Z}^d)^*,$$

with $\mathcal{F}_{\mathbb{B}^c}$ used to denote the $\sigma$-algebra generated by $\{\eta_b \mid b \in \mathbb{B}^c\}$.

For a particular case of a smooth *strictly convex* $V$, Funaki and Spohn [2] have shown (see also [3]) that ergodic infinite-volume Gibbs measures are characterized by their "tilt". Namely, for any linear map $L : \mathbb{R}^d \to \mathbb{R}^m$, there exists a *unique* tempered (finite second moments) $\mu \in \text{ext}\,\mathcal{G}(V)$ with the expectation $\int \eta_b \mu(\mathrm{d}\eta) = L(e)$ for all $b = (x, x+e)$ with any (positively oriented) unit coordinate vector $e$.

In [1], we describe a mechanism leading to a *non-unicity* of measures in $\text{ext}\,\mathcal{G}(V)$ with vanishing tilt, $\int \eta_b \mu(\mathrm{d}\eta) = 0$, for the case of a non-convex $V$. The construction is based on the order-disorder transition proof as introduced in [4]. A simple

case is to consider $d = m = 2$ (actually, in [1] we take $m = 1$) and define the potential $V : \mathbb{R} \to \mathbb{R}$ by

$$(4) \qquad\qquad \mathrm{e}^{-V(t)} = p\,\mathrm{e}^{-\kappa_{\mathrm{O}} t^2/2} + (1-p)\,\mathrm{e}^{-\kappa_{\mathrm{D}} t^2/2}.$$

Here $\kappa_{\mathrm{O}}$ and $\kappa_{\mathrm{D}}$ are positive numbers and $p$ is a parameter taking values in $[0,1]$. For appropriate values of the constants, the graph of $V(|\eta_b|)$, $\eta_b \in \mathbb{R}^2$, defined in this way is as illustrated in the accompanying figure. The indexing of the coupling constants suggests the names: "O" for *ordered* and "D" for *disordered*. Indeed, one can show that, for $\kappa_{\mathrm{O}}$ and $\kappa_{\mathrm{D}}$ sufficiently distinct from each other, there occurs a first order transition between the "ordered" and "disordered" phases with $\eta_b$ either narrowly concetrated or more widely spread, respectively, around its vanishing mean. Namely, one can prove the following claim [1].
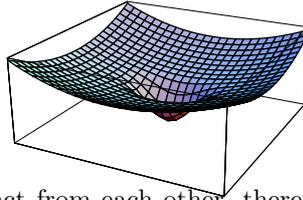
**Theorem 9.** *For $\kappa_{\mathrm{O}} \gg \kappa_{\mathrm{D}}$, there exists a number $p_{\mathrm{t}} \in (0,1)$ such that, for $V$ with $p = p_{\mathrm{t}}$, the set $\mathrm{ext}\,\mathcal{G}(V)$ contains two distinct measures $\mu_{\mathrm{ord}}$ and $\mu_{\mathrm{dis}}$ with zero mean and distinct fluctuation size,*

$$(5) \qquad\qquad \int |\eta_b|^2 \mu_{\mathrm{ord}}(\mathrm{d}\eta) \ll \int |\eta_b|^2 \mu_{\mathrm{dis}}(\mathrm{d}\eta).$$

One can actually show [5] that these measures have distinct stiffness: in an appropriate scaling limit, they converge to distinct Gaussian limits.

Using the particular form (4) of $V$, one can rewrite the Gibbs weight

$$(6) \qquad \prod_b \big( p\,\mathrm{e}^{-\kappa_{\mathrm{O}} |\eta_b|^2/2} + (1-p)\,\mathrm{e}^{-\kappa_{\mathrm{D}} |\eta_b|^2/2} \big) = \prod_b \mathrm{e}^{-\kappa_b |\eta_b|^2/2} \rho(\mathrm{d}\kappa_b)$$

with the measure $\rho(\mathrm{d}\kappa_b) = p\delta_{\kappa_{\mathrm{O}}}(\mathrm{d}\kappa_b) + (1-p)\delta_{\kappa_{\mathrm{D}}}(\mathrm{d}\kappa_b)$. Consider now an extended Gibbs measure, joint in the variables $(\eta_b, \kappa_b)$, whose $\eta$-marginal is a Gibbs measure of the original model. Employing the fact that the extended measure on a torus is *reflection positive* and using *chessboard estimates*, one can show that a typical configuration has the bonds of either overwhelmingly ordered or overwhelmingly disordered type ($\kappa_b = \kappa_{\mathrm{O}}, \kappa_{\mathrm{D}}$). Observing that the former is certainly the case for $p$ close to 1, while the latter for $p$ small, one argues that the expected fraction of occupied bonds has to undergo a jump for some $p = p_{\mathrm{t}}$. This fact leads to a possibility of constructing the measures $\mu_{\mathrm{ord}}$ and $\mu_{\mathrm{dis}}$ from the $\eta$-marginal of the limiting torus measure by taking the limits $p \to p_{\mathrm{t}}$ from above and below.

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# Minimum principles for characterizing the trajectories and microstructural evolution of dissipative systems

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(joint work with A. Mielke, S. Conti)

In their classical formulation, the class of evolutionary problems considered in [1] take place in a Banach space $Y$ and their strong form is the doubly nonlinear differential inclusion

$$(1a) \qquad 0 \in \partial\Psi(\dot{u}(t)) + D\mathcal{E}(t, u(t)),$$

$$(1b) \qquad u(0) = u_0,$$

where $\Psi : Y \to \mathbb{R}_\infty := \mathbb{R} \cup \{\infty\}$ is a convex dissipation potential; $\mathcal{E} : Y \to \mathbb{R}_\infty$ is an energy function; $\partial\Psi$ is the subdifferential of $\Psi$, representing the system of dissipative forces; $D\mathcal{E}$ is the Fréchet derivative of $\mathcal{E}$, representing the conservative force system; and time $t$ varies in the interval $[0, T]$. Equation (1a) establishes a balance between dissipative forces and conservative forces, and the trajectory $u(t)$ of the system is the result of this balance and of the initial condition (1b). In [1], the evolutionary problem (1) is reformulated in a weaker form enabling the consideration of systems where $\mathcal{E}$ is not differentiable or not even lower semi-continuous, thus allowing for solutions that may exhibit *evolving microstructures*. This reformulation is accomplished by expressing (1) in variational form, i. e., by identifying a functional whose minimizers represent *entire trajectories* of the system. Specifically, suppose that we are given the state $u_0$ of the system at time $t_0 = 0$ and wish to approximate the solution $u_n$ at times $t_n = n\triangle t$, $n = 1, \ldots, N$. A *sequence* of minimum problems that delivers consistent approximations to the solution of the continuous-time evolutionary problem (1) is

$$(2) \qquad \inf_{u_{n+1} \in Y} F_{n+1}(u_{n+1}; u_n), \quad n = 0, \ldots, N - 1,$$

where

$$(3) \qquad F_{n+1}(u_{n+1}; u_n) = \triangle t \, \Psi\left(\frac{u_{n+1} - u_n}{\triangle t}\right) + \mathcal{E}(t_{n+1}, u_{n+1}) - \mathcal{E}(t_n, u_n)$$

is an incremental functional that combines energy and kinetics. In addition, in (2) it is tacitly understood that the problems are solved *causally*: problem $n = 0$ is solved first with initial conditions $u_0$ in order to computed $u_1$; subsequently, problem $n = 1$ is solved to compute $u_2$, taking the solution $u_1$ of the preceding problem as initial condition; and so on. We note that the datum $-\mathcal{E}(t_n, u_n)$ is added to (2) so that kinetic and energy terms are of the same order in $\triangle t$. We wish

instead to collect the sequence (2) of incremental problems into a single minimum problem for the entire trajectory $u = \{u_1, \ldots, u_N\}$. In the theory of optimization, a standard device for combining multiple objective functions is supplied by the concept of *Pareto optimality*. In this spirit, a candidate functional on trajectories is

$$\text{(4)} \qquad \mathcal{I}(u; \lambda) = \sum_{n=0}^{N-1} \lambda_{n+1} F_{n+1}(u_{n+1}; u_n)$$

where $\lambda = \{\lambda_1, \ldots, \lambda_N\}$ are positive *Pareto weights*. However, it order to ensure causality it is necessary to choose the weights in such a way that the minimization of the single functional $\mathcal{I}(u; \lambda)$ with respect to the entire trajectory $u$ is equivalent to the sequential solution of the incremental problems (2). This is accomplished by introducing the ordering: $\lambda_1 \gg \lambda_2 \gg \ldots$, which accords disproportionately larger importance to the first incremental problem relative to the second; to the second incremental problem relative to the third, and so on. More specifically, we may accomplish this causal ordering by considering a sequence of positive weights $\lambda_1^\epsilon > \lambda_2^\epsilon > \ldots$ parameterized by a real parameter $\epsilon \geq 0$ and such that

$$\text{(5)} \qquad \lim_{\epsilon \to 0} \frac{\lambda_{n+1}^\epsilon}{\lambda_n^\epsilon} = 0.$$

Inserting these weights into $\mathcal{I}(u; \lambda)$ gives

$$\text{(6)} \quad \mathcal{I}(u; \lambda^\epsilon) = \sum_{n=0}^{N-1} \lambda_{n+1}^\epsilon \left\{ \Psi\left( \frac{u_{n+1} - u_n}{\triangle t} \right) + \frac{\mathcal{E}(t_{n+1}, u_{n+1}) - \mathcal{E}(t_n, u_n)}{\triangle t} \right\} \triangle t.$$

Suppose, in addition, that there is a function $\lambda_\epsilon > 0$ such that

$$\text{(7)} \qquad \lambda_n^\epsilon = \lambda_\epsilon(t_n).$$

Inserting (7) into (6) we obtain

$$\text{(8)} \; \mathcal{I}(u; \lambda^\epsilon) = \sum_{n=0}^{N-1} \lambda_\epsilon(t_{n+1}) \left\{ \Psi\left( \frac{u_{n+1} - u_n}{\triangle t} \right) + \frac{\mathcal{E}(t_{n+1}, u_{n+1}) - \mathcal{E}(t_n, u_n)}{\triangle t} \right\} \triangle t.$$

This functional may be regarded as a time discretization of the continuous-time functional

$$\text{(9)} \qquad \mathcal{I}(u; \lambda_\epsilon) = \int_0^T \lambda_\epsilon \left[ \Psi(\dot{u}) + \frac{d}{dt} \mathcal{E}(t, u) \right] dt,$$

Alternatively, an integration by parts gives the functional in the from

$$\text{(10)} \qquad \mathcal{I}(u; \lambda_\epsilon) = \lambda_\epsilon(T) \mathcal{E}(T, u(T)) + \int_0^T \left[ \lambda_\epsilon \Psi(\dot{u}) - \dot{\lambda}_\epsilon \mathcal{E}(t, u) \right] dt,$$

up to an inconsequential additive constant. For the particular choice of weights

$$\text{(11)} \qquad \lambda_\epsilon(t) = \mathrm{e}^{-t/\epsilon},$$

$$\text{(12)} \qquad \mathcal{I}_\epsilon(u) = \mathrm{e}^{-T/\epsilon} \mathcal{E}(T, u(T)) + \int_0^T \mathrm{e}^{-t/\epsilon} \left[ \Psi(\dot{u}) + \frac{1}{\epsilon} \mathcal{E}(t, u) \right] dt.$$

We now may regard the one-parameter family of minimum problems:

$$(13) \qquad \inf_{u \in \mathbb{Y}, \; u(0)=u_0} \mathcal{I}_\epsilon(u),$$

where $\mathbb{Y}$ is some suitable space of trajectories $u : [0,T] \to Y$, as a continuous-time version of the sequence (2) of incremental problems. We refer to $\mathcal{I}_\epsilon(u)$ as the *energy-dissipation functional*. In particular, one would expect that the limit of $\triangle t \to 0$ of (2) and the limit of $\epsilon \to 0$ of (13) characterize the same trajectories, and that these trajectories satisfy (1) in some appropriate sense.

A class of problems that is amenable to effective analysis concerns *rate-independent systems* for which the dissipation potential $\Psi$ is homogeneous of degree 1 [1]. A striking first property of rate-independent problems is that all minimizers $u^\epsilon$ of $\mathcal{I}_\epsilon$ satisfy energy balance independently of the value of $\epsilon$. Under suitable coercivity assumptions it is then possible to derive *a priori* bounds for $u^\epsilon$ which likewise are independent of $\epsilon$, with the result that it is possible to extract convergent subsequences and find limiting functions $u$. Under very general assumptions we show that all such limits satisfy the *energetic formulation* for rate-independent systems of Mielke *et al.* (see, e. g., the survey [2] and references therein). Moreover, we show that if $(\Psi_k)_{k \in \mathcal{N}}$ continuously converges to $\Psi$ and $\mathcal{E}_k$ $\Gamma$-converges to $\mathcal{E}$ in the weak topology of a Banach space, then the accumulation points of the family $(u_{\epsilon,k})_{\epsilon>0, k \in \mathcal{N}}$ for $\epsilon, 1/k \to 0$ solve the associated limiting energetic formulation.

In addition, the one-dimensional system characterized by a dissipation function

$$(14) \qquad \Psi(u_t) = \int_0^a \frac{1}{2} u_t^2 dx,$$

and an energy function

$$(15) \qquad \mathcal{E}(u) = \begin{cases} \displaystyle\int_0^1 |u_{xx}| dx, & \text{if } |u_x| = 1 \text{ a. e.,} \\ +\infty, & \text{otherwise.} \end{cases}$$

and the two-dimensional system characterized by a dissipation function

$$(16) \qquad \Psi(u_t) = \int_{(0,1)^2} \frac{1}{2} u_t^2 dx$$

and an energy function

$$(17) \qquad \mathcal{E}(u) = \begin{cases} \displaystyle\int_{(0,1)^2} |\nabla^2 u| dx, & \text{if } \nabla u \in K \text{ a. e.} \\ +\infty, & \text{otherwise,} \end{cases}$$

with $K = \{(0, \pm 1), (\pm 1, 0)\}$, are amenable to analysis [3]. In particular, the relaxation and optimal time scaling properties of the systems can be characterized analytically at fixed $\epsilon$. The systems thus provide examples of evolving microstructure that can effectively be understood within the energy-dissipation functional framework.

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