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Interplay of Analysis and Probability in Physics

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Abstract. The main purpose of this workshop was to foster interaction between researchers in the fields of analysis and probability with the aim of joining forces to understand difficult problems from physics rigorously. 52 researchers of all age groups and from many parts of Europe and overseas attended. The talks and discussions evolved around five topics on the interface between analysis and probability. The main goal of the workshop, the systematic encouragement of intense discussions between the two communities, was achieved to a high extent.

Mathematics Subject Classification (2000): 60xx, 70xx, 74xx, 82xx.

Introduction by the Organisers

Developments in the last few years have shown that hard problems from physics can be tackled by combining tools from analysis and probability. The main goal of this workshop was therefore to bring together researchers working on selected topics on the interface between analysis and probability and to encourage intensive discussions between them. The topics chosen evolve around a rigorous understanding of complex physical systems, some of which contain random inputs. The participants were mostly well-known researchers in either field with a profound interest in the other, but also a number of younger scientists at the beginning of their career attended. The particular mixture of people encouraged a high degree of interaction.

The workshop was a continuation of an Oberwolfach workshop held in December 2008. The general aim and spirit of the two workshops were similar, but the

concrete topics of the two workshops had only a limited overlap, and apart from the organisers just seven researchers attended both workshops.

The schedule of the workshop was as follows. Each of the five days was devoted to one of the topics (1) Optimal transport, (2) Discrete-to-continuum transitions in systems out of equilibrium, (3) Diffusion and mass transport in inhomogeneous media, (4) Surfaces and interface evolutions, (5) Phase transitions in many-body systems. In the morning, a 60-minutes talk with survey character was delivered by a senior scientist, followed by two to five research talks of 40 minutes each. One further session was devoted to nine 5-minute talks by young scientists. In this way, almost all younger participants had the opportunity to present their work. Every talk was followed by a discussion and a number of questions from the audience.

The main goal of the workshop was remarkably well achieved. Evidence for this were intense cross-community discussions and an unusually high number of questions and remarks after every talk coming equally from representatives of both fields. The interaction between researchers in analysis and probability was much more intense than in the 2008 workshop. This may be due to the choice of the topics and of the participants, but we believe it mainly reflects the success of this workshop series (and other recent events) in closing the gap between the two research communities.

We now turn to a short description of the main contributions of the workshop. The first day was opened with a survey by Felix Otto on the interaction between gradient flows and hydrodynamic limits. Then Giuseppe Savaré gave an overview of the recent developments in metric-measure theory, and its connection to heat flows and entropy gradient flows. Yann Brenier presented a remarkable derivation of a one-dimensional compressible Navier-Stokes equation from a system of random walkers that is replaced in ordered sequence at every time step. Max von Renesse discussed stochastic analysis on the Wasserstein space and the Wasserstein diffusion. Marco di Francesco presented an extension of the Wasserstein gradient flow theory to a class of partial differential equation with singular potential. Finally Wilfrid Gangbo described recent developments in the theory of Vlasov systems.

On the second day Frank den Hollander presented recent results on the behaviour of a random copolymer near an interface between two immiscible solvents, showing variational characterizations of the phase diagram. Jean-Dominique Deuschel demonstrated a method to construct Markov chains approximating a given diffusion process with non-symmetric diffusion coefficients. Gero Friesecke presented a novel application of optimal transport theory in the context of density functional theory. Lorenzo Bertini explained how to extend the Donsker-Varadhan large deviation principle for the empirical measure by considering also the empirical flow of a Markov process. Pierre Mathieu described a remarkable scaling limit for a random walk in a trap environment, and Greg Pavliotis presented a deterministic coupled system consisting of a classical particle in contact with a heat bath, where the heat bath is modelled as a wave equation.

The third day started with Errico Presutti highlighting some aspects of two types of phase transitions for classical many-body systems with potentials of

Lennard-Jones type: solid-gas and fluid-gas. He put some emphasis on low-temperature aspects and connected up with optimality results derived at zero temperature. An approximate description of the first type of transitions at coupled low temperature and low density, using a large-deviation ansatz, was presented by Sabine Jansen. Daniel Ueltschi considered probability measures on the set of partitions, which are motivated by the study of the interacting Bose gas, but have many more interesting applications in statistical physics.

The fourth day was opened by Claudio Landim, who presented and compared the hydrodynamics of three interesting classes of random particle dynamics with exclusion and explained the differences in the structure of the dynamics and how they are reflected in the nature of the limiting differential equation. Then Cristian Giardinà described the concept of duality and an example application, in which the duality permits the exact solution of a class of interacting diffusions. Tony Lelièvre explained two methods to use coarse-graining in metastable systems for the efficient calculation of averages. This was followed by our session for young researchers, before Dirk Blömker addressed the question of stabilization of stochastic partial differential equations by additive noise, with applications to the Swift-Hohenberg equation and a Burgers' equation.

On the final day Andrey Piatnitski explained homogenization for certain types of parabolic operators with subdiffusive, diffusive and superdiffuse rescaling of the time variable. Aaron Yip presented a crystal growth model, in particular the peculiarities at the interface of the arising optimal shape, the Wulff shape. Antal Jarai gave a survey of the Markovian dynamics of sandpile models and analysed minimal recurrent configurations on unboundedly growing graphs. Omar Lakkis described an approach to error estimates in stochastic partial differential equations in L^∞- and L^p-norms, with applications to the Allen-Cahn equation with additive noise. Finally, Karsten Matthies used a collision tree approach to derive a simplified Boltzmann equation from a system of deterministic particles with random positions and annihilation dynamics.

Workshop: Interplay of Analysis and Probability in Physics

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Abstracts

Heat flows, Dirichlet forms and gradient estimates in Metric Measure Spaces

Giuseppe Savaré
(joint work with Luigi Ambrosio and Nicola Gigli)

Let (X,d) be a length, complete, and separable metric space endowed with a measure $\mathfrak{m}\in\mathcal{P}_2(X)$ (the space of Borel probability measures with finite quadratic moment) with dense support. The Wasserstein distance in $\mathcal{P}_2(X)$ is defined by

$$W_2^2(\mu,\nu):=\min\int \mathsf{d}^2(x,y)\,\mathrm{d}\pi(x,y)\quad\text{for every }\mu,\nu\in\mathcal{P}_2(X),\tag{1}$$

where the minimum is taken among all the couplings $\pi\in\mathcal{P}_2(X\times X)$ having marginals μ and ν. $\mathrm{Ent}_{\mathfrak{m}}:\mathcal{P}_2(X)\to[0,+\infty]$ denotes the Entropy functional

$$\mathsf{Ent}_{\mathfrak{m}}(\rho):=\int_X u\log u\,\mathrm{d}\mathfrak{m}\quad\text{if }\rho=u\mathfrak{m}\ll\mathfrak{m},\qquad \mathsf{Ent}_{\mathfrak{m}}(\rho)=+\infty\quad\text{if }\rho\not\ll\mathfrak{m}.\tag{2}$$

The metric-measure space $(X,\mathsf{d},\mathfrak{m})$ has *Ricci curvature bounded from below* by $K\in\mathbb{R}$ according to Sturm [14] and Lott-Villani [8] (LSV-spaces), if every couple $\mu_0,\mu_1\in D(\mathsf{Ent}_{\mathfrak{m}})=\{\rho:\mathsf{Ent}_{\mathfrak{m}}(\rho)<\infty\}$ can be connected by a *minimal geodesic* curve $s\mapsto\mu_s\in D(\mathsf{Ent}_{\mathfrak{m}})$, $s\in[0,1]$, such that for every $s,t\in[0,1]$

$$W_2(\mu_s,\mu_t)=|s-t|W_2(\mu_0,\mu_1),\tag{3a}$$

$$\mathsf{Ent}_{\mathfrak{m}}(\mu_s)\le(1-s)\mathsf{Ent}_{\mathfrak{m}}(\mu_0)+s\mathsf{Ent}_{\mathfrak{m}}(\mu_1)-\frac{K}{2}s(1-s)W_2^2(\mu_0,\mu_1).\tag{3b}$$

If (3b) holds along *any* geodesics in $\mathcal{P}_2(X)$ connecting μ_0 to μ_1 we say that $(X,\mathsf{d},\mathfrak{m})$ satisfies the *strong* $\mathrm{CD}(K,\infty)$-condition.

When (X,d) is a complete Riemannian manifold with metric tensor g, the above condition is equivalent [15] to the pointwise lower bound $\mathbf{Ric}_{\mathsf{g}}\ge K\,\mathbf{I}$. In this framework, let $u_t:=H_tu$ be the flow solving the Heat equation in $X\times(0,\infty)$

$$\partial_t u-\Delta u=0,\quad\lim_{t\downarrow0}u_t=u\in L^2_{\mathfrak{m}}(X),\tag{4}$$

associated to the Laplace-Beltrami operator Δ. At the level of probability measures, the corresponding flow $\mathsf{H}_t:\rho\in\mathcal{P}_2(X)\mapsto\rho_t\in\mathcal{P}_2(X)$, i.e. $\mathsf{H}_t\rho=(H_tu)\mathfrak{m}$ if $\rho=u\mathfrak{m}$, satisfies the contraction estimate [1, 7, 16]

$$W_2(\mathsf{H}_t\rho,\mathsf{H}_t\sigma)\le\mathrm{e}^{-Kt}W_2(\rho,\sigma)\quad\text{for every }\rho,\sigma\in\mathcal{P}_2(X),\tag{5}$$

and the *Evolution variational inequality* (EVI, in short)

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac12W_2^2(\rho_t,\sigma)+\mathrm{Ent}_{\mathfrak{m}}(\rho_t)+\frac12\mathrm{e}^{-2Kt}W_2^2(\rho_t,\sigma)\le\mathrm{Ent}_{\mathfrak{m}}(\sigma)\quad\forall\,\sigma\in D(\mathrm{Ent}_{\mathfrak{m}}).\tag{6}$$

This deep connection between the Heat flow, the Entropy, and the Wasserstein distance have been discovered by Otto [12] in the Euclidean setting and further

studied by many authors, see e.g. [1, 16]. In particular [11, 13, 10] exploited the link of (3b), (5) and (6) with the Bochner inequality

$$\frac{1}{2}\Delta|\nabla u|^2_{\mathsf{g}} - \langle \nabla u, \Delta_{\mathsf{g}} \nabla u\rangle_{\mathsf{g}} = |\nabla\nabla u|^2_{\mathsf{g}} + \mathbf{Ric}_{\mathsf{g}}(\nabla u, \nabla u) \geq K|\nabla u|^2_{\mathsf{g}}. \tag{7}$$

It is also well known that (7) lies at the core of the Bakry-Emery Γ-calculus for the Dirichlet forms [5] and it is equivalent to the pointwise gradient estimate

$$\left|\nabla H_t u\right|^2 \leq \mathrm{e}^{-2Kt}\, H_t\big(|\nabla u|^2\big). \tag{8}$$

In general metric-measure spaces the Heat flow H_t can be defined as the $L^2_{\mathfrak{m}}(X)$-gradient flow of the Cheeger energy [6, 2] $\mathsf{Ch} : L^2_{\mathfrak{m}}(X) \to [0,\infty]$

$$\mathsf{Ch}(u) := \frac{1}{2}\inf\left\{\liminf_{h\to\infty}\int |\nabla u_h|^2\,\mathrm{d}\mathfrak{m} : u_h \in \mathrm{Lip}(X),\ \int_X |u_h - u|^2\,\mathrm{d}\mathfrak{m} \to 0\right\}, \tag{9}$$

where for a Lipschitz function $u : X \to \mathbb{R}$ we set $|\nabla u|(x) := \limsup_{y\to x} \frac{|u(y)-u(x)|}{\mathsf{d}(x,y)}$. Since Ch is a convex (but no more quadratic, in general) and lower semicontinuous functional, the (possibily nonlinear) Laplace operator $\Delta : D(\Delta) \subset L^2_{\mathfrak{m}}(X) \to L^2_{\mathfrak{m}}(X)$ can be defined as the minimal selection of the subdifferential of Ch and it generates a unique flow (see e.g. [4]) $H_t : L^2_{\mathfrak{m}}(X) \to D(\Delta)$ such that $u_t := H_t\, u$ satisfy the Cauchy problem (4). Notice that

$$H_t \quad \Leftrightarrow \quad \Delta \text{ is linear} \quad \Leftrightarrow \quad \mathsf{Ch} \text{ is quadratic.} \tag{10}$$

It should be clear that the LSV-notion of lower Ricci curvature bound is too weak, if one hopes to extend all these properties and relationships to a more general class of metric measure spaces: in fact LSV-spaces include arbitrary Banach and Finsler spaces, in which the Heat equation is generally nonlinear [9]. In [3] we introduce a more restrictive intrinsic notion to lower Ricci bound that rules out Finsler geometries and still enjoys nice stability, tensorization and locality features.

Definition ($\mathrm{RCD}(K,\infty)$-spaces [3])**.** $(X,\mathsf{d},\mathfrak{m})$ has *Riemannian Ricci curvature bounded from below by* $K \in \mathbb{R}$ if for every $\rho \in \mathcal{P}_2(X)$ there exists a locally Lipschitz curve $\rho_t = \mathsf{H}_t\rho \in \mathcal{P}_2(X)$, $t \geq 0$, satisfying (6) with $\lim_{t\downarrow 0}\rho_t = \rho$.

Theorem 1 (Equivalent formulations [3])**.** *$(X,\mathsf{d},\mathfrak{m})$ is a $\mathrm{RCD}(K,\infty)$-space if and only if one of the following two conditions hold:*

(RCD1) *The Heat flow H_t is linear in $L^2_{\mathfrak{m}}(X)$ (or, equivalently, Ch is quadratic, according to (10)) and $(X,\mathsf{d},\mathfrak{m})$ is a strong $\mathrm{CD}(K,\infty)$-space.*

(RCD2) *The Heat flow H_t is linear and satisfies the contraction property (5).*

Theorem 2 (Heat flow, Dirichlet form, Brownian motion [3])**.** *If $\rho = u\mathfrak{m} \in \mathcal{P}_2(X)$ with $u \in L^2_{\mathfrak{m}}(X)$, then $\mathsf{H}_t\rho = (H_t u)\mathfrak{m}$.*

Lipschitz regularization and pointwise estimates: *the Heat flow satisfies the strong Feller regularization property $H_t(L^\infty_{\mathfrak{m}}(X)) \subset \mathrm{Lip}(X)$ for $t > 0$ and the pointwise gradient estimate*

$$\left|\nabla(H_t u)\right|^2 \leq \mathrm{e}^{-2Kt} H_t\big(|\nabla u|^2\big) \quad \textit{for every } u \in \mathrm{Lip}(X). \tag{11}$$

Dirichlet form and distance: Ch *is a strongly local Dirichlet form admitting* Γ*-calculus and* d *coincides with the Lipschitz distance induced by* Ch.

Markov process: *there exists a unique (in law) Markov process* $\{\mathbf{X}_t\}_{t\geq 0}$ *with continuous sample paths in* $[0,\infty)$ *and transition probabilities* $\mathsf{H}_t\,\delta_x$*, i.e.*

$$\mathbb{P}\big(\mathbf{X}_{s+t}\in A|\mathbf{X}_s=x\big)=\big(\mathsf{H}_t\delta_x\big)\,(A)\quad \textit{for every } s,t\geq 0,\ A \textit{ Borel.} \tag{12}$$

Theorem 3 (Structural properties [3])**.**

Stability: *if* $(X_n,\mathsf{d}_n,\mathfrak{m}_n)$ *are* $\mathrm{RCD}(K,\infty)$*-spaces converging to* $(X,\mathsf{d},\mathfrak{m})$ *in the measured-Gromov-Hausdroff sense as* $n\uparrow\infty$*, then* $(X,\mathsf{d},\mathfrak{m})$ *is* $\mathrm{RCD}(K,\infty)$.

Tensorization: *if* $(X_i,\mathsf{d}_i,\mathfrak{m}_i)$*, are* $\mathrm{RCD}(K,\infty)$ *then also* $(X_1\times X_2,\mathsf{d},\mathfrak{m}_1\otimes\mathfrak{m}_2)$ *is* $RCD(K,\infty)$ *where* $\mathsf{d}^2((x_1,x_2),(y_1,y_2)):=\mathsf{d}_1^2(x_1,y_1)+\mathsf{d}_2^2(x_2,y_2)$.

Locality: *let* $\{X_i\}_{i\in I}$ *be a finite or countable cover of* X *made of closed sets with* $\mathfrak{m}(X_i)>0$, $\mathfrak{m}(\partial X_i)=0$. *If* X *is nonbranching then* $(X,\mathsf{d},\mathfrak{m})$ *is* $RCD(K,\infty)$ *iff each* $(X_i,\mathsf{d},\mathfrak{m}_i)$ *is* $RCD(K,\infty)$*, where* $\mathfrak{m}_i:=\mathfrak{m}^{-1}(X_i)\mathfrak{m}\llcorner X_i$.

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Integration of a 1D compressible Navier-Stokes model by random walks with delayed elastic collisions

Yann Brenier

Deriving the Navier-Stokes equation of compressible gases from simple systems of interacting particles with noise, without going back to the Maxwell-Boltzmann kinetic theory, seems a natural goal. This can be achieved in the elementary and not really physical following situation: we consider only one space variable, we neglect the temperature equation, we assume that both the pressure and the viscosity depend linearly on the density. More precisely, we consider the CNSE (compressible NS equations):

$$\begin{aligned} \partial_t(\rho v) + \partial_x(\rho v^2 + \lambda\epsilon\rho)) &= \epsilon\partial_x(\rho\partial_x v), \\ \partial_t\rho + \partial_x(\rho v) &= 0, \end{aligned} \tag{1}$$

where λ, ϵ are positive constants. The corresponding system of particles can be described as follows. Given a uniform time step $h > 0$, we consider K particles of unit mass on the real line with positions $X_{n,k}$ at time $t = nh$, ordered in increasing order for $k = 1, \cdots K$. We introduce an auxiliary variable $Z_{n,k}$. At each time step, we first move each particle to the new position

$$\hat{X}_{n+1,k} = (1 + h\lambda)X_{n,k} + hZ_{n,k} + \sqrt{2\epsilon h}N_{n,k} \tag{2}$$

where $N_{n,k}$ is a given sequence of independent random numbers, with expectation 0 and unit variance. After this step, which includes a random walk, the positions of particles are (in general) no longer in increasing order. Then, we sort them in increasing order an obtain the updated positions $X_{n+1,k}$. Finally, we update the $Z_{n,k}$ by setting

$$Z_{n+1,k} = (1 - \lambda h)Z_{n,k} - h\lambda^2 X_{n,k}. \tag{3}$$

[Observe that the sorting step can be interpreted in terms of elastic collisions 'with delay". It is well known that 1D elastic collisions of particles of same mass are ineffective since they just amount to exchanging labels. Indeed, 1D colliding particle just exchange their velocities after an elastic collision. However, if two colliding particles wait for the next time step $(k + 1)h$ before exchanging their velocities ("delayed elastic collisions), the effect will be equivalent to the sorting of positions in increasing order.]

Our convergence analysis is done without stochastic analysis, by substituting $(-1)^k$ for the random number $N_{n,k}$. This choice introduces enough "mixing", thanks to the reordering step. In addition, we consider the case of 1-space periodic solutions of the CNSE, which requires a little of care for the reordering step, but largely simplifies the PDE part of the proof.

The proof starts with a "material" formulation of the CNSE. We denote by $X(t,a)$ the "material" positions of the fluid parcels, so that

$$\partial_t X(t,a) = v(t, X(t,a)), \quad \partial_a X(t,a)\rho(t, X(t,a)) = 1.$$

Next, we introduce

$$Z(t,a) = -\lambda X(t,a) + \partial_t X(t,a) + \partial_a(1/\partial_a X(t,a)) \tag{4}$$

and get for Z, after elementary calculations (using our special choice of pressure and viscosity), an elementary ODE:

$$\partial_t Z + \lambda(Z + \lambda X) = 0. \tag{5}$$

So, we get an evolution set of equations for (X, Z) where the only non-trivial part corresponds to the non-linear scalar evolution operator

$$\partial_t X(t,a) + \partial_a(1/\partial_a X(t,a)) \tag{6}$$

which is nothing but the "material" version of the plain heat operator acting on the density ρ

$$\partial_t \rho - \partial^2_{xx}\rho \tag{7}$$

Then the consistency of the discrete model of particles becomes rather clear as a space-time discretization of the "material" version of the CNSE, where $(X_{n,k}, Z_{n,k})$ approximates $(X(t,a), Z(t,a))$: the random walk simulates the heat part of the equations, while the reordering step enforces the constraint $\partial_a X(t,a) \geq 0$ at the discrete level.

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Nonlocal interaction PDEs, gradient flows and optimal transport

Marco Di Francesco

(joint work with José A. Carrillo, A. Figalli, T. Laurent, D. Slepçev)

We consider a class of partial differential equations of the form

$$\partial_t \mu = \operatorname{div}(\mu \nabla W * \mu), \tag{1}$$

posed on the whole space $\mathbb{R}^d$ with arbitrary dimension d. In the equation (1), $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ the space of probability measure with finite second moment. The interaction potential W is even, continuous, radial $W(x) = w'(|x|)$, locally attractive at $x = 0$ i. e. $w'(r) > 0$ on $r \in (0, r_0)$, and λ-convex i. e. $W(x) + \lambda\frac{|x|^2}{2}$ convex for some $\lambda \in \mathbb{R}$.

The model (1) is the continuum counterpart of the interacting N-particle system

$$\dot{X}_i(t) = -\sum_{j\neq i,\ j=1}^{N} m_j \nabla W(X_i(t) - X_j(t)), \qquad i = 1, \dots, N, \tag{2}$$

which finds several applications in statistical physics [6], population biology [8], material sciences [5], and sociology [9]. A slightly different version of those models incorporates linear or nonlinear diffusion effects, see [6].

A typical situation occurring in some of the above mentioned context is the *total collapse* of the measure μ in a finite time, i. e. $\mu(t) = \delta_{x_c}$ for $t \geq t^*$ with t^* depending on the initial condition and x_c being the center of mass of the system (preserved in time). Such situation is reminiscent of what happens in chemotaxis modeling, see [7]. Such property can be easily proved for finite particles (2) as follows: let $I \in \{1, \dots, N\}$ be such that $X_I(t)$ is the particle with largest distance to x_c, assume w. l. o. g. $x_c = 0$ (I can vary in time, but it has only a finite number of jumps, since particles stick together when they collide). A direct computation shows that the quantity $|X_I(t)|$ decreases in time (it is immediate if we assume the ratio $w'(r)/r$ is decreasing, otherwise this requires some more work, see [2]), and it collapses to zero at time

$$t^* = \int_0^{X_I(0)} \frac{1}{w'(r)} dr.$$

In particular, if a non-Osgood type condition is assumed for W, namely that the ratio $1/w'(r)$ be integrable at $r = 0$, then $t^* < +\infty$. It can be easily proven that t^* only depends on the radius of the support of the empirical measure $\mu = \sum_{j=1}^{N} m_j \delta_{X_j}$ at time $t = 0$. In particular, t^* does not depend on N.

In the proposed work, a general existence and uniqueness theory for (1) is presented, which allows (for the first time) to include potentials with *pointy singularity* at the origin. Such theory is an extension of the Wasserstein gradient flow theory developed in [1]. As a further improvement of such theory, we can also include potentials with quadratic repulsive growth at infinity. The main technical point needed to perform this task is the rigorous characterization of the velocity field $v(x) = \int_{\mathbb{R}^d} \nabla W(x - y) d\mu(y)$ in the continuity equation (1). Clearly, when the measure μ concentrates, v is not well defined in case of pointy potentials W, i. e. ∇W discontinuous at $x = 0$. Such difficulty reflects the technical issue in the theory [1] to define the *subdifferential* of the interaction energy functional

$$\mathcal{W}[\mu] = \frac{1}{2} \iint_{\mathbb{R}^{2}d} W(x - y) d\mu(x) d\mu(y), \qquad \mu \in \mathcal{P}_2(\mathbb{R}^d). \tag{3}$$

We propose the formula

$$\partial^0 \mathcal{W}[\mu](x) = \int_{x\neq y} \nabla W(x - y) d\mu(y)$$

for the minimal subdifferential (i. e. element of the subdifferential with minimal $L^2(d\mu)$-norm) of $\mathcal{W}$ on μ. We then exploit the λ-convexity assumption to prove

existence and uniqueness of gradient flow solutions to (1) in the sense of [1] with the property

$$d_W(\mu_1(t), \mu_2(t)) \leq e^{\lambda t} d_W(\mu_1(0), \mu_2(0)), \tag{4}$$

for two solutions μ_1 and μ_2. Here d_W denotes the 2-Wasserstein distance.

The main advantage of our approach is that it allows to include singular measures in our theory. It was in fact known in [3] that $L^1 \cap L^\infty$ solutions to (1) blow up in finite time, but it was not clear how to continue solutions after blow up.

As a very simple application of our theory, we can prove that the total collapse property stated above for particles can be easily proven for *all* compactly supported measure solutions in $\mathcal{P}_2$. We use an atomization technique due to [4], which consists in approximating an initial measure μ_0 with a finite set of particles $\mu_0^N = \sum_{j=1}^N m_j \delta_{X_j}$ such that $d_W(\mu_0, \mu_0^N)$ is arbitrarily small. Then, the stability property (4) gives

$$d_W(\mu(t), \mu^N(t)) \leq e^{\lambda t} d_W(\mu_0, \mu_0^N),$$

and on substituting $t = t^*$, with t^* being the time of total collapse of μ^N to a delta, we get that the solution $\mu(t)$ to (1) with initial condition μ_0 becomes a single delta at x_c in finite time.

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Particle dynamics with interactions on the real line

Wilfrid Gangbo
(joint work with Yann Brenier, Giuseppe Savaré, and Michael Westdickenberg)

In a joint work with Adrian Tudorascu, we extended the weak KAM theory to infinite dimensional systems such as the Vlasov system. Let $W \in C^2(\mathbb{R}^d)$ be periodic such that $W \leq W(0)$ and let μ_0 an initial probability measure on $\mathbb{R}^d \times \mathbb{R}^d$. The Vlasov system we consider consists in finding a path $t \to \mu_t$ on the set $\mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d)$ of probability measures of bounded second moments, distributional solution of

$$\partial_t \mu + \nabla_x \cdot (p\mu) = \nabla_p \cdot (\mu \nabla W * \varrho). \tag{1}$$

Here, ϱ is the spatial marginal of the probability measure μ. We showed that given $\varrho_0 \in \mathcal{P}_2(\mathbb{R}^d)$ and $c \in \mathbb{R}^d$ we can choose $u_0 : \mathbb{R}^d \to \mathbb{R}^d$ square integrable with respect to ϱ_0 such that the solution of (1) starting at

$$\mu_0 = \varrho_0(dx)\delta_{p-u_0(x)}(dp)$$

satisfies

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \Big| \frac{x}{t} + c \Big|^2 \mu_t(dx, dp) \leq \frac{C}{\sqrt{t}}.$$

Thus,

$$\lim_{t \to \infty} \int_{\mathbb{R}^d \times \mathbb{R}^d} \Big| \frac{x}{t} + c \Big|^2 \mu_t(dx, dp) = 0.$$

In fact, with A. Tudorascu, we showed existence of a path $t \to \varrho_t \in \mathcal{P}_2(\mathbb{R}^d)$ and $u_t : \mathbb{R}^d \to \mathbb{R}^d$ square integrable with respect to ϱ_t, such that

$$\mu_t = \varrho_t(dx)\delta_{p-u_t(x)}(dp).$$

As a consequence the pair (ϱ, u) is a distributional solution of

$$\partial_t \varrho + \nabla_x \cdot (\varrho u) = 0, \qquad \partial_t(\varrho u) + \nabla_x(\varrho u \otimes u) = -\varrho \nabla W * \varrho. \tag{2}$$

This naturally raises the following question: given $\varrho_0 \in \mathcal{P}_2(\mathbb{R}^d)$ and $u_0 : \mathbb{R}^d \to \mathbb{R}^d$ square integrable with respect to ϱ_0, can we find $t \to (\varrho_t, u_t)$ starting at (ϱ_0, u_0) and satisfying (2). When $d = 1$, in a joint work with Y. Brenier, G. Savaré and M. Westdickenberg, we developed a theory which answers the question in the general case

$$\partial_t \varrho + \partial_x(\varrho u) = 0, \qquad \partial_t(\varrho u) + \partial_x(\varrho u^2) = \varrho f_\varrho. \tag{3}$$

In (3) the expression $-W' * \varrho$ has been replaced by a more general expression f_ϱ, such that f_ϱ is a Borel function defined ϱ–almost everywhere. We explained how (3) can be described by a differential inclusion on the space of transport maps. We proved a stability result for solutions of this system and its connection with sticky-particle systems.

Variational description of random polymers

Frank den Hollander
(joint work with Erwin Bolthausen and Alex Opoku)

We consider a random copolymer near a selective interface separating two solvents. The configurations of the copolymer are directed paths that can make i.i.d. excursions of finite length above and below the interface. The excursion length distribution is assumed to have a tail that is logarithmically equivalent to a power law with exponent $\alpha \geq 1$. The monomers carry i.i.d. real-valued types whose distribution is assumed to have zero mean, unit variance, and a finite moment generating function. The interaction Hamiltonian rewards matches and penalizes mismatches of the monomer types and the solvents, and depends on two parameters: the interaction strength $\beta \geq 0$ and the interaction bias $h \geq 0$. We are interested in the behavior of the copolymer in the limit as its length tends to infinity.

The quenched free energy per monomer $(\beta, h) \mapsto g^{\text{que}}(\beta, h)$ has a phase transition along a quenched critical curve $\beta \mapsto h_c^{\text{que}}(\beta)$ separating a localized phase, where the copolymer stays close to the interface, from a delocalized phase, where the copolymer wanders away from the interface. We derive *variational formulas* for both these quantities. We compare these variational formulas with their analogues for the annealed free energy per monomer $(\beta, h) \mapsto g^{\text{ann}}(\beta, h)$ and the annealed critical curve $\beta \mapsto h_c^{\text{ann}}(\beta)$, both of which are explicitly computable. This comparison leads to:

(1) A proof that $g^{\text{que}}(\beta, h) < g^{\text{ann}}(\beta, h)$ for all $\alpha \geq 1$ and (β, h) in the annealed localized phase.
(2) A proof that $h_c^{\text{ann}}(\beta/\alpha) < h_c^{\text{que}}(\beta) < h_c^{\text{ann}}(\beta)$ for all $\alpha > 1$ and $\beta > 0$.
(3) A proof that $\liminf_{\beta \downarrow 0} h_c^{\text{que}}(\beta)/\beta \geq K_c$ with $K_c = (1+\alpha)/2\alpha$ for $\alpha \geq 2$ and $K_c \in [B(\alpha)/\alpha, (1+\alpha)/2\alpha]$ for $1 < \alpha < 2$ with $B(\alpha) > 1$.
(4) An estimate of the total number of times the copolymer visits the interface in the interior of the quenched delocalized phase.
(5) An identification of the asymptotic frequency at which the copolymer visits the interface in the quenched localized phase.

The copolymer model has been studied extensively in the literature. The goal of the present work is to open up a window with a variational view and to settle a number of long-standing open problems.

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Markov chain approximation to non-symmetric diffusions with bounded coefficients

Jean-Dominique Deuschel
(joint work with Takashi Kumagai)

We consider a diffusion operator in divergence form

$$LF(x) = \sum_{i,j=1}^{d} \partial_{x_i}\Big(a^{i,j}(x)\partial_{x_j}F(x)\Big)$$

which is uniformly elliptic and bounded: the coefficients a_{ij} are real measurable functions such that

$$|a_{ij}(x)| \le C_1, \quad \sum_{i,j} a_{i,j}(x)\xi_i\xi_j \ge \epsilon \sum_i \xi_i^2.$$

The corresponding (non symmetric) Dirichlet form is then given by

$$E(F,G) = \sum_{ij} \int_{\mathbb{R}^d} \partial_{x_i}F(x)a_{ij}(x)\partial_{x_j}G(x)\,dx.$$

It is well known that non-negative solutions to the calorific (parabolic) equation satisfy the scale-invariant parabolic Harnack principle, in particular the associated heat kernel have some Hölder regularity with both upper and lower Gaussian bounds.

The aim of this paper is to construct the associated diffusion process by an approximation with finite range random walks on the rescaled lattice $S_n = \frac{1}{n}\mathbb{Z}^d$.

In case of a symmetric diffusion matrix

$$a_{ij} = a_{ji}$$

[SZ] give an explicit construction based on a discrete analogy of the Nash-Moser-De Giorgi theory for symmetric uniformly irreducible walks. In particular they derive the Hölder regularity for the corresponding heat kernels. Further results allowing unbounded jump ranges converging to symmetric processes with both diffusions and jumps have been obtained in [BK] and [BKU]. However such estimates for non-symmetric Markov chains were still unknown.

Our first objective is to identify the class of non-symmetric walks satisfying a scale invariant parabolic Harnack inequality as the class of Markov chains with bounded cycle decompositions. In this class of processes on S_n, the (rescaled) Dirichlet form is given by

$$E_n(F,G) = \sum_{\gamma_n \in \Gamma_n} n^{2-d} E_{\gamma_n}(F,G)$$

where

$$E_{\gamma_n}(F,G) = \sum_{x_i \in \gamma_n} \big(F(x_i) - F(x_{i+1})\big)\big(G(x_i) - G(x_0)\big).$$

Here $\gamma_n = (x_0, x_1, ..., x_\ell = x_0)$ is a collection of oriented cycles of length $\ell(\gamma_n) = \ell \geq 2$ and $\alpha_n(\gamma_n) > 0$ are the weights of the cycles. When the length of the cycles is at most two, we have a symmetric chain.

We make the following assumptions: bounded weight, bounded cycle length and bounded range:

$$\alpha_n(\gamma_n) \leq M_1, \quad \ell(\gamma_n) \leq M_2, \quad \text{range}(\gamma_n) \equiv \max_{x_i} |x_i - x_{i+1}| \leq \frac{M_3}{n}.$$

Also we assume that the chain is uniformly irreducible, i.e. the corresponding time discrete chain $\{X_k^{(n)}, k = 0, 1, ...\}$ satisfies, for each $x \in S_n$ and unit vector e_i there exist $k = k(x, \pm e_i) \leq N$ with

$$P(X_k^{(n)} = x \pm e_i/n | X_0^{(n)} = x) \geq \delta.$$

Our first result then shows that the scale-invariant parabolic Harnack principle holds, and we thus get gaussian heat kernel estimates for with Hölder continuity.

In particular tightness follows from these estimates and the next question we address deals with convergence issue: find conditions which guarantee the convergence of the heat kernels of the Markov chains to the heat kernel of the non-symmetric diffusion process. It is well known, that convergence of the corresponding Dirichlet forms:

$$\lim_{n\to\infty} E_n(F, G) = E(F, G) = \sum_{ij} \int \partial_{x_i} F(x) a_{ij}(x) \partial_{x_j} G(x)\, dx, \quad F, G \in C^1(\mathbb{R}^d),$$

does not suffice.

Instead we rewrite the Dirichlet form of the Markov chain as

$$E_n(F, G) = n^{-d} \sum_{x,y \in S_n} \sum_{i,j=1}^{d} \nabla_n^i F(x) b_{i,j}^n(x, y) \nabla_n^i G(y)$$

for adequate coefficients $b_{ij}^n(x, y)$, where $\nabla_n^i F(x) = n\big(F(x + e_i/n) - F(x)\big)$ is the discrete partial derivative and we set

$$a_{ij}^n(x) = \sum_y b_{ij}^n(x, y).$$

Then local convergence of a^n to a in $L^1(\mathbb{R}^d)$:

$$\lim_{n\to\infty} \int_K |a_{ij}^n(x) - a_{ij}(x)| dx = 0, \qquad \forall K \text{ compact set of } \mathbb{R}^d$$

imply convergence of the heat kernels and weak convergence of the Markov chain to the diffusion process.

Finally we return to the original question: for given bounded uniformly elliptic matrix a_{ij} how to construct the Markov chain converging to the diffusion process. In view of the above, all we need is to find the corresponding bounded cycle decomposition such that the coefficient of the discretized Dirichlet form converges locally in $L^1(\mathbb{R}^d)$.

Our construction is very explicit and could easily be numerically implemented. We use a simple two scale analysis, with piecewise constant approximation of the diffusion matrix at mesoscopic scale $n^{-1/2}$. Next we deal with the symmetric $\tilde{a}(x)$ and the antisymmetric $\hat{a}(x)$ part of the matrix $a(x)$.

For the antisymmetric part we create for each $i \neq j$ with $\hat{a}_{i,j}(x) > 0$ rotational cycles $\gamma_{ij}(x)$ to nearest neighbors of length $8L$ passing through the corners

$$x,\ x - 2L(e_i/n),\ x - 2L(e_i/n) - 2L(e_j/n),\ x - 2L(e_j/n)$$

with weight

$$\alpha_n(\gamma_{ij}(x)) = \frac{\hat{a}_{ij}(x)}{2L}.$$

For the symmetric part, we first bring the matrix in diagonalized form,

$$\sum_{i,j} \tilde{a}_{i,j}(x)\xi_i\xi_j = \sum_{i=1}^{d} \lambda_i(x)\big(V_i(x)\cdot\xi\big)^2$$

and then introduce the cycles of length two

$$\gamma_i(x) = (x, x + V_i(x)/n, x)$$

with weight

$$\alpha_n(\gamma_i(x)) = \lambda_i(x)$$

We use the Feshbach map in order to bring the matrix in diagonalized form without having to compute the eigenvalues and eigenvectors of the matrix $\tilde{a}(x)$.

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Density functional theory and optimal transportation with Coulomb cost

Gero Friesecke

(joint work with Codina Cotar and Claudia Klüppelberg)

We recently discovered that in a natural scaling limit, the celebrated Hohenberg-Kohn density functional from electronic structure theory reduces to an optimal transport problem. Our work thereby links density functional theory (DFT), which is a quantum mechanical theory of electrons and constitutes a large and very active research area in physics and chemistry, for the first time to optimal transportation theory, which has recently become a very active area in mathematics.

Informal connection Quantum mechanics – DFT – Optimal transport. The chemical behaviour of atoms and molecules is described accurately, at least in principle, by quantum mechanics. Quantum mechanics for the electrons in a molecule boils down to a partial differential equation for a function $\Psi \in L^2(\mathbb{R}^{3N}, \mathbb{C})$, where N is the number of electrons and where, for simplicity, we ignore spin. The Born formula says that $|\Psi(x_1, .., x_N)|^2$ is the joint probability density of positions $x_1, .., x_N \in \mathbb{R}^3$. To simulate chemical behaviour, approximations are needed. This is because of a 'curse of dimension' phenomenon: Discretizing $\mathbb{R}$ by 10 gridpoints means that $\mathbb{R}^{3N}$ has 10^{3N} gridpoints. E.g., CO_2 has 22 electrons, giving rise to an unfeasible 10^{66} gridpoints.

DFT [PY95] is *the* standard approximation to quantum mechanics in simulations with more than a dozen or so electrons, and was introduced by Hohenberg, Kohn and Sham in the 1960s. It approximates quantum mechanics via a closed eq. for the marginal density

$$\rho_1(x_1) = \int |\Psi(x_1, .., x_N)|^2 dx_2 \cdots dx_N.$$

All one-point marginals are equal, since $|\Psi|^2$ is symmetric in the x_i, by the Pauli principle.

The full Schrödinger equation can be reformulated as hierarchy of eq's: for ρ_1 in terms of the pair density $\rho_2(x_1, x_2) = \int |\Psi(x_1, .., x_N)|^2 dx_3 \cdots dx_N$, for ρ_2 in terms of ρ_3, etc. DFT models, i.e. closed eq's for ρ_1, can be viewed as semi-empirical models of the pair density ρ_2 in terms of its marginal ρ_1. Mathematicians may not be familiar with DFT, but its inventor Walter Kohn received the 1998 Nobel Prize in Chemistry, and DFT is routinely used in physics, chemistry, materials science and molecular biology to predict binding energies and molecular geometries.

There are many different DFT models. The simplest is based on a statistical independence (or mean field) assumption, $\rho_2 = \rho_1 \otimes \rho_1$, and goes back to Thomas and Fermi in 1927. Early modern DFT computations used the local density approximation, in which correlations are modelled via electron gas theory. More accurate functionals were developed, among others, by Becke, Lee, Yang, Parr, Perdew, Wang, Burke, and Ernzerhof. While the accuracy of the best functionals (compared to more exact quantum mechanical computations or experimental data) is impressive in many situations, designing functionals with further improved accuracy continues to be the goal of a great deal of research in physics and chemistry. Mathematically, the best DFT models used in practice have no rigorous connection to full quantum mechanics, and an accompanying lack of systematic improvability.

Informally, the connection quantum mechanics – DFT – optimal transport is as follows [CFK11]. For $N = 2$ electrons, and in the semiclassical limit $\hbar \to 0$, the following closure relation between single-particle density and pair density becomes

exact:

$$\rho_2 \quad = \quad \text{solution of an optimal transport problem with Coulomb cost and equal marginals } \rho_1.$$

The optimal transport problem is:

$$\min_{\gamma\in\mathcal{P}(\mathbb{R}^6)} \int_{\mathbb{R}^6} \frac{1}{|x-y|} d\gamma(x,y) \text{ s/to right and left marginal } \rho_1, \tag{1}$$

where $\mathcal{P}(\mathbb{R}^d)$ denotes the probability measures on $\mathbb{R}^d$. Note that while ρ_1 and ρ_2 depend on $\hbar$ and on the molecule-dependent external potential v appearing in the full quantum mechanical equation for the electronic wave function Ψ, the closure relation is universal.

Mathematically, the cost function in the above OT problem has two novel features, cost decreases with distance, and has a singularity on diagonal. On the other hand, there is one simplifying feature, namely equal marginals.

The above closure relation can be generalized to an arbitrary number of particles; one obtains a many-marginal optimal transport problem [CFK12].

Using methods from OT theory, especially of [GM96], one can show that the solution to problem (1) is unique, and given by an optimal map, $\rho_2(x,y) = \rho_1(x)\delta_{T(x)}(y)$ (i.e., the Kantorovich problem is equivalent to the corresponding Monge problem).

Rigorous connection Quantum mechanics – DFT – OT. The 'exact' (non-relativistic, Born-Oppenheimer) quantum mechanical ground state energy of a molecule is given by

$$E_0 = \inf_{\Psi\in\mathcal{A}_N} E[\Psi] \tag{2}$$

where, ignoring spin for simplicity, $\mathcal{A}_N$ consists of the functions in the Sobolev space $H^1(\mathbb{R}^{3N})$ which are antisymmetric in the coordinates $x_1,..,x_N \in \mathbb{R}^3$ and satisfy $||\Psi||_{L^2} = 1$, and $E[\Psi] = T[\Psi] + V_{ee}[\Psi] + V_{ne}[\Psi]$ with

$$T = \frac{\hbar^2}{2}\int_{\mathbb{R}^{3N}} |\nabla\Psi|^2,\ V_{ne} = \int_{\mathbb{R}^{3N}} \sum_i v(x_i)|\Psi|^2,\ V_{ee} = \int_{\mathbb{R}^{3N}} \sum_{i<j} \frac{1}{|x_i - x_j|}|\Psi|^2$$

(kinetic energy, electron-nuclei interaction energy, and electron repulsion energy; $\hbar$ is Planck's constant and $v : \mathbb{R}^3 \to \mathbb{R}$ is a molecule-specific external potential). As noticed by Hohenberg and Kohn, the non-universal part of the energy only depends on the single-particle density $\rho_1^\Psi =: \rho^\Psi$:

$$V_{ne}[\Psi] = \int \sum_i v(x_i)|\Psi(x_1,..,x_N)|^2 = N\int_{\mathbb{R}^3} v(x)\,\rho^\Psi(x)\,dx.$$

One can therefore partition the minimization in (2) into a double minimization, first over Ψ subject to fixed ρ, then over ρ:

$$\begin{aligned} E_0 &= \inf_{\Psi}\Big(T[\Psi]+V_{ee}[\Psi]+N\int v(r)\,\rho^{\Psi}(r)\,dr\Big) \\ &= \inf_{\rho}\underbrace{\inf_{\Psi\mapsto\rho}\Big(T[\Psi]+V_{ee}[\Psi]\Big)}_{=:F^{HK}[\rho]}+N\int v(r)\,\rho(r)\,dr. \end{aligned}$$

The functional F^{HK} is known after its inventors as the *Hohenberg-Kohn functional*; the above constrained-search definition of it is due to M.Levy. The domain of F^{HK} consists of the image $\mathcal{R}_N$ of the set $\mathcal{A}_N$ under the map $\Psi \mapsto \rho_\Psi$. Our "closure relation" can now be rigorously stated as follows:

Theorem 1. *For $N = 2$, and all $\rho \in \mathcal{R}_N$,*

$$\lim_{\hbar\to 0} F^{HK}[\rho] = E^{OT}[\rho],$$

where $E^{OT}[\rho]$ is the optimal cost of (1) as a function of the marginal ρ.

The difficulty in proving this is a regularity issue. Any wavefunction Ψ whose square is the optimal plan γ of the limiting OT problem is far from having finite kinetic energy (it is not even in L^2), and can therefore not be used as a trial function in the variational definition of F^{HK}. But smoothing the optimal plan γ destroys the marginal constraint. We therefore developed a novel technique to restore the marginal constraint after smoothing while at the same time keeping the cost under control.

Exactly soluble examples. To get a basic feeling of the behaviour of the OT problem (1), let us look at some exactly integrable examples. For these, the Coulombic form of the cost is not essential, one needs that $c = c(|x-y|)$ is positive, decreasing with distance, and, crucially, convex in the distance. Rigorously deriving the formulae below relies on the methods of [MC99]. Shortly after giving the talk, I learned that the formulae in examples 2) and 3) are known, on grounds of physical intuition and formal arguments, in the physics literature [Se99, SGS07]. Recall that the optimal measure is of the "Monge" form $\gamma(x,y) =) = \rho_1(x)\delta_{T(x)}(y)$.

1) ρ_1=uniform measure on [0,1]. Then $T(x) = x + 1/2$ for $x < 1/2$, and $x - 1/2$ for $x > 1/2$. That is to say, T rigidly switches the two halves of the interval.

2) $\rho_1 \in L^1(\mathbb{R})$, positive. With a denoting the median of ρ_1, for $x < a$ we have

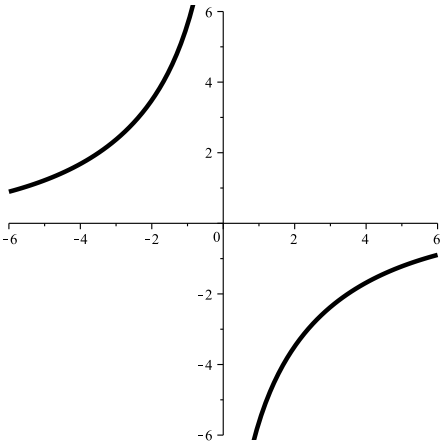
$$\int_{-\infty}^{x}\rho_1 = \int_{a}^{T(x)}\rho_1,$$

and similarly for $x > a$. Thus T maps the interval left of the median to the interval right of the median, while re-stretching it appropriately so as to satisfy the constraint that T pushes forward $\rho_1|_{\{x<a\}}$ to $\rho_1|_{\{x>a\}}$.

3) $\rho_1 \in L^1(\mathbb{R}^d)$, positive, radially symmetric. Then for $r > 0$, $e \in S^{d-1}$

$$T(r\mathbf{e}) = -t(r)\mathbf{e}$$

with $t(r)$ determined by $\int_{-\infty}^{r} |S_s^{d-1}|\rho_1(s)\,ds = \int_0^{t(r)} |S_s^{d-1}|\rho_1(s)\,ds$. This means, in particular, that T maps lines through the origin to themselves, and points on such a line to points on the opposite side of the origin.



The plot shows the optimal map T restricted to a line through the origin, for $\rho_1(x) = const\, e^{-|x|}$, $x \in \mathbb{R}^3$.

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Scaling limits of trap models, K-processes and aging

Pierre Mathieu

In [3], we introduced K-processes as scaling limits for the following model of random walk with traps, originally studied by Bouchaud in [1] as a toy model for spin glasses. Let S be a finite set and consider the Markov chain which, when

sitting at site x, waits for an exponentially distributed time of mean $\tau(x)$ and then jumps to another point in S chosen with uniform probability.

It turns out that, when the rates $(\tau(x)\,;\, x \in S)$ are chosen at random according to an i.i.d. law with a power tail, then this (properly rescaled) trap model converges to a scaling limit, as the cardinality of S tends to infinity.

More generally, K-processes are Markov processes on the one point compactification of $\mathbb{N}$ with a single instantaneous state (the 'infinity'). Besides appearing as scaling limits of random walks as above, they can also be directly constructed, either in analytic terms through their Dirichlet forms or by probabilistic means, via Poisson processes. We also gave a characterization of K-processes through their entrance laws. In words, a K-process is characterized by its holding time when sitting at some point in $\mathbb{N}$ and its sojourn time at 'infinity', plus the property that, when starting at 'infinity', it enters any finite set with a uniform law. Of course, in order to fulfill this last requirement, starting from 'infinity', a K-process must almost surely perform an infinite number of jumps before any positive time. (It is a Markov process of the fourth kind in P. Lévy's classification.)

The results in [3] have later been extended to the dynamics of the Random Energy Model in [4] and K-processes were also used in [6] to describe scaling limits of sequences of random walks on a large torus.

We recently revisited scaling limits of trap models 'à la Bouchaud' in [7] with two objectives. We introduce a non homogeneous version of K-processes (when the entrance law is not uniform anymore) which is related to the scaling limit of trap models in which the probability to jump to a point $x \in S$ is not uniform anymore but proportional to $\tau(x)^a$, for some asymmetry parameter $a > 0$.

The second result in [7] is a new description of the way the limiting K-process jumps when starting from infinity. This description takes the form of a second scaling limit, as time tends to 0, where the limiting process can be expressed in terms of jumps of subordinators. As a consequence we recover the asymptotics of correlation functions of trap models - the so called 'aging' results - similar to those proved in [2] and [5] by a different method.

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Markovian Approximation of Open Classical Systems

Grigorios A. Pavliotis

We consider the dynamics of a classical particle in one dimension coupled to a heat bath which is at equilibrium at temperature β^{-1}. The full dynamics of the coupled particle/heat bath model is assumed to be Hamiltonian. The heat bath is modeled through a linear wave equation with initial conditions distributed according to the appropriate Gibbs measure. The Hamiltonian of the full dynamics is [KHM97]

$$\mathcal{H}(p,q,\pi,\phi) = \frac{p^2}{2} + V(q) + \frac{1}{2}\int_{\mathbb{R}} \left(|\pi|^2 + |\partial_x \varphi|^2\right) dx + \int_{\mathbb{R}} \varphi(x)\rho(x-q)\, dx. \tag{1}$$

Under the assumption that the potential $V(q)$ is confining, we can approximate the coupling term with (dipole approximation)

$$H_I(q,\varphi) \approx q \int_{\mathbb{R}} \partial_x \varphi(x)\rho(x)\, dx. \tag{2}$$

The equations of motion for (1) with the coupling (2) are

$$\dot{q} = p, \quad \dot{p} = -V'(q) - \int_{\mathbb{R}} \partial_x \varphi(x)\rho(x)\, dx, \tag{3a}$$

$$\partial_t \varphi = \pi, \quad \partial_t \pi = \partial_x^2 \varphi + q\partial_x \rho. \tag{3b}$$

We will use the notation $\phi = (\varphi,\, \pi)$ and

$$\mathcal{A} = \begin{pmatrix} 0 & 1 \\ \partial_x^2 & 0 \end{pmatrix}, \tag{4}$$

and H_E will denote the Hilbert space equipped with the energy norm

$$\langle \phi_1, \psi_2 \rangle = \int_{\mathbb{R}} \left(\partial_x \phi_1(x)\overline{\partial_x \phi_2}(x) + \pi_1(x)\overline{\pi_2}(x)\right) dx \tag{5}$$

where the overbar denotes the complex conjugate. Furthermore, it is convenient to introduce the notation $\alpha = (\alpha_1(x),\, 0) \in H_E$ with $\partial_x \alpha_1(x) = \rho(x)$. We can **formally** write the Gibbs measure with which the initial conditions of the wave equation are distributed in the form

$$\text{“}\mu_\beta(d\phi) = \frac{1}{Z} e^{-\frac{\beta}{2}\|\phi\|^2_{H_E}} \Pi_{x\in\mathbb{R}}\, d\phi.\text{”} \tag{6}$$

We solve equations (3b) and substitute into (3) to obtain the **Generalized Langevin Equation** (GLE) [JP98]

$$\ddot{q} = -V'_{\text{eff}}(q) - \int_0^t \gamma(t-s)\dot{q}(s)\, ds + F(t), \tag{7}$$

where

$$V_{\text{eff}}(q) = V(q) - \frac{1}{2}\lambda^2 q^2, \quad \lambda = \|\rho\|_{L^2}, \tag{8}$$

and

$$\gamma(t) = \left\langle e^{-\mathcal{A}t}\alpha, \alpha \right\rangle . \tag{9}$$

Furthermore, the forcing term $F(t)$ is a mean zero (assuming that $q(0) = 0$) stationary Gaussian stochastic process given by

$$F(t) = \left\langle \phi(0), e^{-\mathcal{A}t}\alpha \right\rangle . \tag{10}$$

Since the initial conditions of the heat bath are distributed according to a Gaussian Gibbs measure, $\phi(0)$ is a Gaussian random field and we can prove the **fluctuation-dissipation theorem**

$$\mathbb{E}(F(t)F(s)) = \beta^{-1}\gamma(t-s). \tag{11}$$

The GLE (7) together with the fluctuation-dissipation theorem is equivalent to the Hamiltonian dynamics (1) with the coupling (2) and random initial conditions for the heat bath variables. The ergodic properties of this system were studied in [JP98].

It was noticed in [EPRB99] that the dynamics (7) can be described by a Markovian system in an extended phase space for particular choices of the coupling function $\rho(x)$; in particular those for which their Fourier transform is a rational function of the form $1/|p(k)|^2$ with $p(k) = \sum_{m=1}^{M} c_m(-ik)^m$ a polynomial with real coefficients and roots in the upper half plane. Under this assumption of such a **Markovian heat bath**, exponentially fast convergence to equilibrium was proved for chains of oscillators coupled to two Markovian heat baths at different temperatures [EPRB99, EH00].

We consider finite dimensional Markovian approximations of the GLE (7). The most general Markovian approximation of (7) is [Kup04]

$$\dot{q}_m(t) = p_m(t), \quad q_m(0) = q(0), \tag{12a}$$

$$\dot{p}_m(t) = -\partial_q V(q_m(t)) + \langle \lambda, z(t) \rangle, \quad p_m(0) = p(0), \tag{12b}$$

$$\dot{z}(t) = -p_m(t)\lambda - \hat{\mathcal{A}}z(t) + \mathcal{G}\dot{W}(t), \quad z(0) \sim \mathcal{N}(0, I), \tag{12c}$$

where $z : \mathbb{R}^+ \mapsto \mathbb{R}^m$, $\lambda \in \mathbb{R}^m$, $\hat{\mathcal{A}}, \mathcal{G} \in \mathbb{R}^{m\times m}$. The fluctuation-dissipation theorem (11) takes the form

$$\mathcal{G}\mathcal{G}^T = \beta^{-1}(\hat{\mathcal{A}} + \hat{\mathcal{A}}^T).$$

The autocorrelation function $\gamma_m(t)$ is

$$\gamma_m(t) = \langle e^{-\hat{\mathcal{A}}t}\lambda, \lambda \rangle,$$

which is similar to (9) but in the above equation $\hat{\mathcal{A}}$ is the generator of a contraction semigroup. Under the assumption $\|\gamma_m(t) - \gamma(t)\|_{L^2} \to 0$ we have that $\mathbb{E}|q_m(t) - q(t)|^2 + \mathbb{E}|p_m(t) - p(t)|^2 \to 0$ over $f$inite time intervals. Furthermore, under appropriate assumptions on $\mathcal{A}$, λ the Markovian dynamics is well defined for $m = +\infty$.

For a confining potential V the dynamics (12) with invariant distribution

$$\rho_\beta(q, p, \mathbf{z}) = \frac{1}{Z} e^{-\beta(H(q,p)+\frac{1}{2}\|\mathbf{z}\|^2)}$$

where $H(p,q) = \frac{1}{2}p^2 + V(q)$. In particular, the invariant distribution is independent of $\mathcal{A}$ and λ.

Consider furthermore the rescaled dynamics

$$\begin{aligned}\dot{q}(t) &= p(t), \quad q(0) = q(0), \quad \dot{p}(t) = -\partial_q V(q(t)) + \frac{1}{\epsilon}\langle \lambda, z(t)\rangle, \quad p(0) = p(0),\\ \dot{z}(t) &= -\frac{1}{\epsilon}p(t)\lambda - \frac{1}{\epsilon^2}\mathcal{A}\, z(t) + \frac{1}{\epsilon}\mathcal{G}\dot{W}(t), \quad z(0) \sim \mathcal{N}(0, I).\end{aligned}$$

Then $\{q, p\}$ converge weakly [OP11] to the solution of the Langevin equation

$$\dot{q} = p, \quad \dot{p} = -\partial_q V(q) - \gamma p + \sqrt{2\gamma\beta^{-1}}\dot{W}, \tag{13}$$

where the friction coefficient γ is given by

$$\gamma = \langle \lambda, (A^T)^{-1}\lambda\rangle.$$

Consider (12) with $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_m)$ and $\mathcal{A}$ diagonal with $\mathcal{A}_{ii} = \alpha_i > 0$. The generator of the dynamics (12) is

$$\begin{aligned}\mathcal{L} &= p\cdot\nabla_q - \nabla_q V(q)\cdot\nabla_p + \sum_{j=1}^{m}\lambda_j z_j(t)\cdot\nabla_p\\ &\quad + \sum_{j=1}^{m}\left(-\lambda_j p\cdot\nabla_{z_j} - \alpha_j z_j\cdot\nabla_{z_j} + \alpha_j\beta^{-1}\Delta_{z_j}\right).\end{aligned}$$

The operator $-\mathcal{L}$ considered in the function space $L^2(\mathbb{R}^{2+m}, e^{-\beta(H(p,q)+\frac{1}{2}\|z\|^2)})$ is hypoelliptic and **hypocoercive** [Vil09]. Using the theory of hypocoercivity we can prove exponentially fast convergence to equilibrium in relative entropy [OP11]. Furthermore, a homogenization theorem can be proved for the case where $V(\cdot)$ is periodic. Finally, the spectrum of the generator $\mathcal{L}$ can be computed explicitly when $V(\cdot)$ is quadratic [OPPS12].

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Some examples of phase transitions

Errico Presutti

I will restrict to "phase transitions of first order with order parameter the [mass] density". This simply means that there is a "forbidden interval" of densities, say (ρ', ρ''), so that if we put a mass $\rho|\Lambda|$ of fluid in a region Λ ($|\Lambda|$ its volume) with $\rho \in (\rho', \rho'')$, ("canonical constraint"), then the fluid separates into a part with density ρ' and another one with density ρ''. It does not exist an equilibrium state with homogeneous density ρ. Thus if we "move in Λ" we go from one phase (with density ρ') to another phase (with density ρ'') and we see a "phase transition".

The notion is quantified in statistical mechanics as follows. Denoting by $\mu_{\beta,\Lambda,N}$ the canonical Gibbs measure in the torus Λ at inverse temperature β and with N particles, we shall say that at the inverse temperature β there is a phase transition with forbidden density interval (ρ', ρ'') if given any $\rho \in (\rho', \rho'')$, for any $\epsilon > 0$:

$$\liminf_{R\to\infty} \liminf_{|\Lambda|\to\infty, N/|\Lambda|\to\rho} \mu_{\beta,\Lambda,N}\Big[q : \int_\Lambda \mathbf{1}_{d[\rho_R(q,r),\{\rho',\rho''\}]>\epsilon} dr \ < \epsilon|\Lambda|\Big] = 1 \tag{1}$$

where $q = (q_1, .., q_N) \in \Lambda^N$; $\rho_R(q, r)$ is the empirical density of q at r on scale R, namely

$$\rho_R(q, r) = \frac{\sum_{i=1}^N \mathbf{1}_{|q_i - r|\le R}}{|B_R|} \tag{2}$$

$|B_R|$ the volume of the sphere of radius R; finally $d[a, A]$ is the distance of a from A.

One of the main goals of statistical mechanics is to prove that for realistic interactions the Gibbs measure has indeed phase transitions in agreement with the phase diagrams exhibited by physical fluids with phase coexistence curves between gas and solid, gas and liquid and liquid and solid. Unfortunately not many progresses have been obtained so far and I shall briefly describe here some of the main results.

The 0 temperature case has been studied by F. Theil, [4], and G. Friesecke et al., [5], proving that for a system of point particles in $\mathbb{R}^2$ with Lennard-Jones interactions there is a forbidden interval $(0, \rho_c)$, $\rho_c > 0$. Ground states with density $\rho \in (0, \rho_c)$ are approximated in a torus Λ by the restriction to a subregion Λ' of Λ of a triangular lattice configuration with density ρ_c and no particles in $\Lambda \setminus \Lambda'$.

The extension to positive temperatures T is still open (no matter how small is T) but there is a well established theory for lattice gases, namely when particles are confined to the lattice $\mathbb{Z}^d$ and at each site there can be at most one particle, see for instance Sinai, [3]. The results are obtained by a classification of all possible deviations from the ground states and proving that with large probability they are small and rare. In the continuum the excitations have a much more complex structure and the techniques developed in the lattice fail.

There are instead results for particles in the continuum regarding the liquid-vapour transition, where instead of perturbing the ground states we perturb the mean field solutions. The theory goes back to Kac and Lebowitz-Penrose, see [2]

and references therein, whose aim was to derive the van der Waals theory in a statistical mechanics context. The hamiltonian in the Kac theory can be written as:

$$H_\gamma(q) = \int_{\mathbb{R}^d} e\big(\rho_{\gamma^{-1}}(q,r)\big)dr \tag{3}$$

where in the original paper by Kac, the energy density is $e(s) = -s^2/2$ and the particles are hard spheres with finite radius. $\gamma > 0$ is called the Kac scaling parameter and the main result was a proof that the free energy density in the limit $\gamma \to 0$ has a flat part at low temperatures indicative of a phase transition. However in the limit $\gamma \to 0$ the hamiltonian $H_\gamma(q)$ is not well defined and this phase transition cannot be attributed to a legitimate system of interacting particles.

The difficulties come from the presence of the hard core constraint. Lebowitz, Mazel and Presutti, [1], have circumvented the problem by studying a model without hard cores and where the energy density is $e(s) = -s^2/2 + s^4/4!$. They have the following theorem.

Theorem 1. *For any $d \geq 2$ there are $0 < \beta_c < \beta_0$ and $\gamma_\beta > 0$, $\beta \in (\beta_c, \beta_0)$ so that for any $\beta \in (\beta_c, \beta_0)$ and $\gamma < \gamma_\beta$ there is a forbidden interval $\rho'_{\beta,\gamma}, \rho''_{\beta,\gamma})$.*

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Cluster size distributions at low temperature and low density

Sabine Jansen

(joint work with Wolfgang König and Bernd Metzger)

Motivated by geometric approaches to the problem of phase transitions, we investigate the cluster size distributions for a system of particles in continous configuration space. The pair potential is attractive and particles are distributed according to a classical Gibbs measure (canonical ensemble). Clusters correspond to groups of particles close in configuration space.

More precisely, consider a system of N particles in a box $\Lambda = [0, L]^d \subset \mathbb{R}^d$. The vector of particle positions is $\boldsymbol{x} = (x_1, \dots, x_N) \in \Lambda^N$. Particles interact via a pair interaction potential $v : [0, \infty) \to \mathbb{R} \cup \{\infty\}$, the total energy is

$$U(x_1, \dots, x_N) = \sum_{1 \le j < k \le N} v(|x_j - x_k|).$$

The basic assumptions on the pair potential are the following:

- There is a $r_{\mathrm{hc}} \ge 0$ such that $v(r) = \infty$ for $r < r_{\mathrm{hc}}$ and $v(r) < \infty$ for $r > r_{\mathrm{hc}}$. At $r = r_{\mathrm{hc}}$, the potential may be finite or infinite.
- The potential is stable: for suitable $B > 0$ and all $N \in \mathbb{N}$ and $\boldsymbol{x} \in (\mathbb{R}^d)^N$, $U(x_1, \dots, x_N) \ge -BN$.
- The potential has a finite range, i.e., v has a compact support.
- v has an attractive "tail": let $b := \sup \mathrm{supp} v$, then there is a $\delta > 0$ such that $v(r) < 0$ for all $r \in (b - \delta, b)$.
- v is continuous in $[r_{\mathrm{hc}}, \infty) \cap (0, \infty)$.

For a given inverse temperature $\beta > 0$, let $\mathbb{P}_{\beta,\Lambda,N}$ be the canonical Gibbs measure on Λ^N. Fix $R > b$, with b the potential range. Draw a line between particles x_j, x_k if they have mutual distance $\le R$. In this way each configuration splits into connected components; we call a connected component with k particles a k-cluster. Let $N_k(\boldsymbol{x})$ be the number of k-clusters and $\rho_{k,\Lambda}(\boldsymbol{x}) := N_k(\boldsymbol{x})/|\Lambda|$. We are interested in the distribution of the vector $(\rho_{k,\Lambda}(\boldsymbol{x}))_{k\in\mathbb{N}}$ under the Gibbs measure $\mathbb{P}_{\beta,\Lambda,N}(\mathrm{d}\boldsymbol{x})$, in the thermodynamic limit $N, |\Lambda| \to \infty$, at fixed β and fixed density $\rho = N/|\Lambda|$.

Theorem 1 (Large deviation principle [4])**.** *Fix $\beta > 0$, $0 < \rho < \rho_{\mathrm{cp}}$, with ρ_{cp} the so-called* close-packing density*. There is a function*

$$f(\beta, \rho, \cdot) : \ \mathbb{R}_+^{\mathbb{N}} \to \mathbb{R} \cup \{\infty\}, \ (\rho_k)_{k\in\mathbb{N}} \mapsto f\big(\beta, \rho, (\rho_k)\big)$$

with support contained in $\sum_{k=1}^{\infty} k\rho_k \le \rho$, such that

$$\frac{1}{N!} \int_{\Lambda^N} e^{-\beta U(\boldsymbol{x})} \mathbf{1}\Big((\rho_{k,\Lambda}(\boldsymbol{x})) \approx (\rho_k)\Big) \mathrm{d}\boldsymbol{x} \approx \exp\Big(-\beta|\Lambda| f(\beta, \rho, (\rho_k))\Big),$$

i.e., $\big(\rho_{k,\Lambda}(\boldsymbol{x})\big)_{k\in\mathbb{N}}$ fulfills a LDP with scale $|\Lambda|$ and rate function

$$J_{\beta,\rho}(\{\rho_k\}) := \beta \left[f\big(\beta, \rho, (\rho_k)\big) - f(\beta, \rho) \right].$$

The rate function is good (lower semicontinuous, compact level sets) and convex. (Product topology on $\mathbb{R}_+^{\mathbb{N}}$.)

Every limiting distribution of the cluster size distribution $(\rho_{k,\Lambda}(\boldsymbol{x}))_{k\in\mathbb{N}}$ will be supported on the set of minimizers of $f(\beta, \rho, \cdot)$. In order to exploit this, we need some information on the rate function.

A first theoretical result is a variational representation of $f(\beta, \rho, (\rho_k))$ as an infimum over shift-invariant point processes. The minimization is under constraints referring to the prescribed density and cluster size distribution; the functional that is minimized is akin to the one from the Gibbs variational principle.

This variational representation allows us to transfer statements on $f(\beta,\rho,\cdot)$ to infinite volume Gibbs measures. For example, $f(\beta,\rho,\cdot)$ has a minimizer (ρ_k) such that $\sum_{k=1}^{\infty} k\rho_k < \rho$ if and only if there is a shift-invariant Gibbs measure with density ρ and with a cluster with an infinite number of particles.

Of more practical use, however, are explicit bounds of the rate function: the distribution of $(\rho_{k,\Lambda})$ is well-approximated by a measure coming from random partitions with multiplicative weights, known in physics as an *ideal mixture*. This approximating measure satisfies a large deviations principle with a rate function of the form

$$f^{\text{ideal}}\big(\beta,\rho,(\rho_k)\big) := \sum_{k=1}^{\infty} k\rho_k f_k^{\text{cl}}(\beta) + (\rho - \sum_{k=1}^{\infty} k\rho_k) f_\infty^{\text{cl}}(\beta) + \beta^{-1}\sum_{k=1}^{\infty}\rho_k(\log\rho_k - 1).$$

The cluster free energies $f_k^{\text{cl}}(\beta)$ are defined in terms of partition functions with a connectivity constraint, and $f_\infty^{\text{cl}}(\beta) = \lim f_k^{\text{cl}}(\beta)$. At low temperature, under suitable assumptions on the potential, they behave approximately like ground state energies, $kf_k^{\text{cl}}(\beta) = E_k + O(\beta^{-1}\log\beta)$. The mixing entropy term $\beta^{-1}\sum_k \rho_k(\log\rho_k - 1)$ is of the order $O(\beta^{-1}\rho)$. Therefore, at low temperature and low density, f^{ideal} can be further approximated by the functional

$$g\big(\beta,\rho,(\rho_k)\big) := \sum_{k=1}^{\infty}\rho_k\big(E_k + \beta^{-1}\log\rho\big) + (\rho - \sum_{k=1}^{\infty} k\rho_k)e_\infty,$$

(here $e_\infty = \lim_k E_k/k$), already encountered in [1].

Theorem 2 (Bounds for the rate function [4])**.** *Under suitable assumptions on v (Hölder continuity, bounds on the minimal and maximal interparticle distance in ground states), there are $C,\beta_0,\rho_0 > 0$ such that for all $\beta \geq \beta_0$, $\rho \leq \rho_0$, $\sum_{k=1}^{\infty} k\rho_k \leq \rho$:*

$$\big|f\big(\beta,\rho,(\rho_k)\big) - g\big(\beta,\rho,(\rho_k)\big)\big| \leq C\rho\beta^{-1}\log\beta.$$

Similar bounds are available for the differences between the minimizers and minima of $f(\beta,\rho,\cdot)$ and $g(\beta,\rho,\cdot)$. Since the functional $g(\beta,\rho,\cdot)$ is linear and easily analyzed, one can deduce a number of statements on the limiting cluster size distributions; in particular, one can prove that in the limit $\beta\to\infty$, $\rho = \exp(-\beta\nu)\to 0$, $\nu > 0$ fixed, particles tend to gather in clusters of a given ν-dependent size.

The bounds can be improved by comparing with the full ideal mixture f^{ideal} instead of the simplified functional g [3].

Thus we have, at low density and low temperature, an *approximate* formula for the free energy$f(\beta,\rho)$ (the minimum of $f(\beta,\rho,\cdot)$). On the other hand, there are *exact* expressions for the free energy and pressure in terms of power series, the Mayer and virial series. The relation between the two approaches can be understood by looking at the low-temperature behavior of the classical expansions.

Theorem 3 (Low temperature behavior of the Mayer coefficients [2])**.**
Let $p(\beta,\mu) := \sup_\rho(\rho\mu - f(\beta,\rho))$ (the pressure*) and $b_k(\beta)$ the coefficients of the*

Mayer expansion $\beta p(\beta,\mu) = \sum_{k=1}^{\infty} b_k(\beta)\exp(\beta k\mu)$. *Then*

$$\forall k \in \mathbb{N}: \; b_k(\beta) = \exp\bigl(-\beta(1+o(1))E_k\bigr) \text{ as } \beta \to \infty.$$

This theorem, in combination with bounds on the free energy, also allows us to deduce a number of new statements on the Mayer and virial expansions, including a soft physical interpretation of the radii of convergence: the radius of the pressure-activity increase corresponds to a fast increase from exponentially small to finite density, and the radius of the pressure-density series corresponds to a cross-over from monatomic to polyatomic gas.

Finally, the combination of the previously described results also yields a theorem on where to look for a low density, low temperature gas-solid phase transition:

Theorem 4 (Where to look for a gas-solid phase transition [2])**.** *Suppose that there is a phase transition at* $\rho_{\mathrm{sat}}(\beta)$ *as* ρ *is varied at fixed* β*. Suppose also that* $\rho_{\mathrm{sat}}(\beta) \to 0$ *as* $\beta \to \infty$*. Then the corresponding chemical potential must satisfy*

$$\mu_{\mathrm{sat}}(\beta) = e_\infty + O(\beta^{-1}\log\beta).$$

The theorem is consistent with the Lee-Yang theorem for lattice gases and with the continuum Widom-Rowlinson model.

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Random partitions in statistical mechanics

Daniel Ueltschi

(joint work with Nicholas M. Ercolani and Sabine Jansen)

We describe a model of spatial random partitions that provides a coupling between several different systems: the ideal Bose gas; the zero-range process; particle clustering in classical systems; and spatial permutations. It can be summarised as a "chain of Chinese restaurants".

Random partitions and Chinese restaurant process. Let $\lambda = (\lambda_1, \dots, \lambda_k)$ denote an integer partition, i.e. a sequence of integers that satisfies $\lambda_1 \geq \lambda_2 \geq \cdots \geq 1$ and $\sum_i \lambda_i = n$. Let $r_j(\lambda)$ be the number of elements equal to j. The relevant probability is

$$\nu_n(\lambda) = \frac{1}{h_n} \prod_{j\geq 1} \frac{1}{r_j(\lambda)!} \Bigl(\frac{\theta_j}{j}\Bigr)^{r_j(\lambda)}.$$

When $\theta_j \equiv 1$, we actually have the uniform measure on random permutations (more precisely, the marginal of this measure with respect to cycle lengths). It is also the invariant measure of the Chinese restaurant process, where n customers enter one-by-one, each customer choosing either a spot to the right of a seated customer, or a new table (all with equal probability). It is well-known that, as $n \to \infty$, we have

$$(\tfrac{\lambda_1}{n}, \tfrac{\lambda_2}{n}, \dots) \to \mathrm{PD}(1),$$

i.e. a random sequence distributed according to Poisson-Dirichlet.

Introducing space. Let X be the space, here a finite or countable set. We assume that we have a Chinese restaurant at each $x \in X$. Let $\boldsymbol{n} = (n_x)_{x\in X}$ denote the total occupation at each site x. We consider now the probability

$$\mathbb{P}_{X,n}(\boldsymbol{n}) = \frac{1}{Z(X,n)} \prod_{x\in X} g(x)^{n_x} h_{n_x}.$$

Here, the function $g(x)$ plays the rôle of an external potential, and h_n is any function of n only (but it will soon be equal to the normalisation of ν_n).

A special case is the ideal Bose gas with n bosons in domain $[0, L]^d$, where $X = \frac{1}{L}\mathbb{Z}^d$ is the Fourier space, and

$$\mathbb{P}(\boldsymbol{n}) = \frac{1}{Z} \prod_{k\in\frac{1}{L}\mathbb{Z}^d} \mathrm{e}^{-4\pi\beta\|k\|^2 n_k}\,.$$

Another special case is the invariant measure of the zero-range process, where a particle at x moves to a random neighbour with rate $\tilde{g}(n_x)$. In this case, $g(x) \equiv 1$ and $h_n = \prod_{i=1}^n \frac{1}{\tilde{g}(i)}$.

Under some conditions, these systems display *Bose-Einstein condensation*: at high density, the typical $\boldsymbol{n}$ has one n_x of order n.

General measure. Let $\boldsymbol{\lambda} = (\lambda_x)_{x\in X}$ denote a sequence of integer partitions indexed by the sites $x \in X$, that satisfies $\sum_{x,i} \lambda_{x,i} = n$. Our probability measure is

$$\mathbb{P}_{X,n}(\boldsymbol{\lambda}) = \frac{1}{Z(X,n)} \prod_{x\in X} \prod_{j\geq 1} \frac{\left(g(x)^j \frac{\theta_j}{j}\right)^{r_j(\lambda_x)}}{r_j(\lambda_x)!}.$$

This is the invariant measure of a chain of Chinese restaurants where customers exit restaurants only to enter a new one, with a suitable rate of departures and a size-biased choice of a table. One easily checks that the marginal on $\boldsymbol{n}$ is the probability above. Also, the conditional measure

$$\mathbb{P}_{X,n}(\boldsymbol{\lambda}|\boldsymbol{n}) = \prod_{x\in X} \nu_{n_x}(\lambda_x)$$

takes a simple form. Results for $\mathbb{P}_{X,n}(\boldsymbol{n})$ and for ν_n can be combined to yield results for $\mathbb{P}_{X,n}(\boldsymbol{\lambda})$.

Marginal on r. Let $\boldsymbol{r} = (r_j)_{j\geq 1}$, where $r_j = \sum_x r_j(\lambda_x)$. The marginal probability is

$$\mathbb{P}_{X,n}(\boldsymbol{r}) = \frac{1}{Z(X,n)} \prod_{j\geq 1} \frac{1}{r_j!} \Big(\frac{\theta_j}{j} \sum_{x\in X} g(x)^j \Big)^{r_j}.$$

A special case is particle clustering [3]. In this case, there is no external potential, $g(x) \equiv 1$, and the parameter θ_j is related to the integral of the Gibbs factor over $j-1$ particles that form a "cluster" around the origin.

Another example is the model of spatial permutations, where the state of the system consists of n positions $x_1, \ldots, x_n$ in a finite box, and a permutation σ of n elements. The probability density is given by

$$\frac{1}{Z} \prod_{i=1}^{n} \mathrm{e}^{-\xi(x_i - x_{\sigma(i)}} \, \mathrm{d}x_1 \ldots \mathrm{d}x_n.$$

With ρ the particle density, the weights are given by

$$\theta_j = \tfrac{1}{\rho} (\, \mathrm{e}^{-\xi} \,)^{*j}(0).$$

Under some conditions, there is a critical density above which macroscopic cycles have the Poisson-Dirichlet distribution [2].

Size of the largest component. We restrict now to the case $g(x) \equiv 1$. Let M be the random variable that represents the size of the largest component,

$$M = \max_{x,i} \lambda_{x,i}.$$

First, we have a law of large numbers.

Theorem 1.

$$\frac{M}{n} \to \max\Big(0, 1 - \sum_{j\geq 1} \theta_j\Big).$$

It is not hard to prove a large deviation principle for finite elements, which reveals that $1 - \sum \theta_j$ represents the fraction of indices in infinite components. This shows that a single macroscopic element may occur, in contrast to the case of spatial permutations. The absence of external potential, $g(x) \equiv 1$, plays an important rôle indeed. If the weights depend on a parameter, there is a phase transition when $\sum \theta_j$ becomes less than 1.

We can characterise the size of the largest component for certain specific forms of the parameters $(\theta_j)_{j\geq 1}$.

Theorem 2. *We suppose that* $\sum \theta_j < 1$.

- *Case* $\theta_j = Cj^{-\alpha}$, $1 < \alpha < 2$. *We have*

$$M = \Big(1 - \sum \theta_j\Big) n + (1 + o(1)) C^{1/\alpha} n^{1/\alpha} Y,$$

where Y *is* α*-stable law.*

- *Case* $\theta_j = Cj^{-\alpha}$, $\alpha \geq 2$, *or* $\theta_j = C\,\mathrm{e}^{-j^\alpha}$, $0 < \alpha < \frac{1}{2}$. *We have*

$$M = \Big(1 - \sum \theta_j\Big) n + (1 + o(1)) \sqrt{n \sum j\theta_j}\; Y.$$

  Here, Y *is equal to a standard normal random variable.*
- *Case* $\theta_j = C\,\mathrm{e}^{-j^\alpha}$, $\frac{1}{2} \leq \alpha < 1$. *We have*

$$M = \Big(1 - \sum \theta_j\Big) n - O(n^\alpha) + (1 + o(1)) \sqrt{n \sum j\theta_j}\; Y,$$

  with Y *a standard normal random variable. The term* $O(n^\alpha)$ *is related to the Cramér series.*

The proof of this theorem involves (i) explicit expressions for the probability of M in terms of ratios of partition functions; (ii) partition functions are given by local limit theorems of suitable i.i.d. random variables, following [1]; (iii) local limit theorems proposed in particular by Nagaev [4].

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Exactly solvable models of heat conduction

Cristian Giardinà
(joint work with Jorge Kurchan, Frank Redig and Kyamars Vafayi)

We review a class of interacting diffusions which have recently been introduced to model transport of heat in a systems in contact with two reservoirs (C. Giardinà, J. Kurchan, F. Redig, *Duality and exact correlations for a model of heat conduction*, J. Math. Phys. **48**, 033301 (2007)). The models can be exactly solved by means of a dual stochastic process made of interacting particles which are absorbed at the boundaries. The construction of the dual process is related to the underlying structure of $SU(1,1)$ algebra. The class of interacting diffusions includes as a special case the KMP model.

Brownian Energy Process. We start with the Brownian Momentum Process introduced in [3]. For a set $\Sigma_m = \{1, \dots, m\}$ with $m \in \mathbb{N}$ and for a graph $G = (V, E)$ with vertex set V and edges set E, we consider the real variables $\{x_{i,\alpha}\}_{i \in V, \alpha \in \Sigma_m}$ and the generator

$$L^{BMP(m)} = \sum_{(i,j)\in E} \sum_{\alpha,\beta=1}^{m} \left(x_{i,\alpha} \frac{\partial}{\partial x_{j,\beta}} - x_{j,\beta} \frac{\partial}{\partial x_{i,\alpha}} \right)^2 . \tag{1}$$

The random variables $x_{i,\alpha}(t)$, evolving with the above generator, represent m momenta per site at time t, and, in the course of evolution, kinetic energy is exchanged between any two momenta in neighboring (i.e. connected by an edge) sites. The energies on each site

$$z_i(t) = \frac{1}{2} \sum_{\alpha=1}^{m} x_{i,\alpha}^2(t)$$

evolve with the generator

$$L^{BEP(m)} = \sum_{(i,j)\in E} z_i z_j \left(\frac{\partial}{\partial z_i} - \frac{\partial}{\partial z_j} \right)^2 - \frac{m}{2}(z_i - z_j) \left(\frac{\partial}{\partial z_i} - \frac{\partial}{\partial z_j} \right) . \tag{2}$$

This is the Brownian Energy Process, BEP(m). The model (2) can actually be defined for a real number $m \in \mathbb{R}$ (i.e. m does not need to be an integer). It is easy to check that the BEP(m) model has stationary measures given by product measures with marginals Gamma distributions with shape parameter $m/2$ and scale parameter $1/\lambda$, i.e. the marginal stationary density at site i is

$$f_\lambda(z_i) = \frac{\lambda^{\frac{m}{2}}}{\Gamma\left(\frac{m}{2}\right)} z_i^{\frac{m}{2}-1} e^{-\lambda z_i} . \tag{3}$$

In particular, for $m = 2$ one has products of Exponential distributions with parameter λ.

Symmetric Inclusion process. The Symmetric Inclusion Process, SIP(m), is an interacting particle systems defined by the generator

$$(L^{SIP(m)} f)(\xi) = \sum_{(i,j)\in E} \xi_i \left(\xi_j + \frac{m}{2} \right) [f(\xi^{i,j}) - f(\xi)] + \xi_j \left(\xi_i + \frac{m}{2} \right) [f(\xi^{j,i}) - f(\xi)] . \tag{4}$$

Here $\{\xi_i\}_{i \in V}$ are integer variables counting the number of particles at every site i of the graph. Given the configuration $\xi = (\xi_1, \dots, \xi_{|V|})$, we denote by $\xi^{i,j}$ the configuration obtained from ξ by removing one particle at i and placing it at j.

One can easily check that product measures with marginals given by Negative Binomials, i.e. with marginal probability mass function at site i given by ($0 \le p \le 1$)

$$\nu_p(\xi_i) = (1-p)^{\frac{m}{2}} \frac{\Gamma(\frac{m}{2} + \xi_i)}{\Gamma(\frac{m}{2})} \frac{p^{\xi_i}}{\xi_i!} , \tag{5}$$

are reversible, and therefore stationary, measures of the SIP(m) process. In particular, for $m = 2$ one has marginal Geometric distributions with parameter $1 - p$.

Duality. Let $\{X(t)\}_{t\geq 0}$ and $\{Y(t)\}_{t\geq 0}$ be two stochastic processes. We say that they are dual with duality function $D(\cdot,\cdot)$ if the following relation hold for all (x, y) and all times t

$$\mathbb{E}_x(D(X(t), y)) = \mathbb{E}_y(D(x, Y(t))) \; . \tag{6}$$

On the left-hand side we have expectation with respect to the $X(t)$ process initialized at x, while on the right-hand side we have expectation with respect to the $Y(t)$ process initialized at y.

Theorem: The process $\{z(t)\}_{t\geq 0}$ with generator $L^{BEP(m)}$ and the process $\{\xi(t)\}_{t\geq 0}$ with generator $L^{SIP(m)}$ are dual, with duality functions

$$D(z, \xi) = \prod_{i\in V} z_i^{\xi_i} \frac{\Gamma(\frac{m}{2})}{\Gamma(\frac{m}{2} + \xi_i)} \tag{7}$$

Proof: Duality is a consequence of the fact that the generator of the BEP(m) process and the generator of the SIP(m) process correspond to the same abstract operator $L_{(m)}$ in two different representations. The abstract operator is given by the ferromagnetic quantum spin chain on the graph G, with spins satisfying the $SU(1, 1)$ algebra. Namely,

$$L_{(m)} = \sum_{(i,j)\in E} \left(\mathcal{K}^+_{(m),i}\mathcal{K}^-_{(m),j} + \mathcal{K}^-_{(m),i}\mathcal{K}^+_{(m),j} - 2\mathcal{K}^o_{(m),i}\mathcal{K}^o_{(m),j} + \frac{m^2}{8} \right) \tag{8}$$

where the spins $\left\{\mathcal{K}^+_{(m),i}, \mathcal{K}^-_{(m),i}, \mathcal{K}^o_{(m),i}\right\}_{i\in V}$ satisfy the $SU(1, 1)$ commutation relations:

$$[\mathcal{K}^o_{(m),i}, \mathcal{K}^\pm_{(m),j}] = \pm\delta_{i,j}\mathcal{K}^\pm_{(m),i} \qquad\qquad [\mathcal{K}^-_{(m),i}, \mathcal{K}^+_{(m),j}] = 2\delta_{i,j}\mathcal{K}^o_{(m),i} \tag{9}$$

The $SU(1, 1)$ algebra admit the following two families (labelled by m) of infinite dimensional representations:

$$\begin{cases} \mathcal{K}^+_{(m),i} = z_i \\ \mathcal{K}^-_{(m),i} = z_i\,\partial^2_{z_i} + \frac{m}{2}\partial_{z_i} \\ \mathcal{K}^0_{(m),i} = z_i\,\partial_{z_i} + \frac{m}{4} \end{cases} \qquad \begin{cases} K^+_{(m),i}|\xi_i\rangle = \left(\xi_i + \frac{m}{2}\right)|\xi_i + 1\rangle \\ K^-_{(m),i}|\xi_i\rangle = \xi_i|\xi_i - 1\rangle \\ K^o_{(m),i}|\xi_i\rangle = (\xi_i + m)\,|\xi_i\rangle \end{cases} \tag{10}$$

The BEP(m) generator is obtained when writing the abstract operator (8) in the representation with second order differential operators; the SIP(m) generator is obtained when writing the abstract operator (8) in the representation with infinite dimensional matrices. The duality functions (7) are found by imposing on each site that the action of the two representations on $D(z_i, \xi_i)$ is the same.

Applications and perspectives. As an application, the BEP(1) process was considered in [3] as a model of heat conduction: a chain with N sites was coupled to two heat reservoirs (modeled by Ornstein-Uhlenbeck process) at different temperatures. The dual process is then a SIP(1) process with absorbing boundaries. A general expression for the energy moments in the stationary state was obtained and solved for the energy covariance. Correlations functions were proved to be positive in general in [5]. In [4] it was shown that if one start from a chain with $m = 2$ and consider an instantaneous thermalization limit of the $BEP(2)$ model, then the KMP model [1] is recovered.

Among the open problem we mention: i) the construction of duality between an asymmetric version of inclusion process $ASIP_q(m)$ and brownian energy process $ABEP_q(m)$. Following the scheme developed in [4] this should involve the deformed quantum group $SU_q(1,1)$; ii) a full ergodic theory of SIP/BEP model; iii) the explicit solution for the stationary measure for models with reservoirs, akin to the exclusion process.

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Mathematical analysis of probabilistic numerical algorithms used in molecular dynamics

Tony Lelièvre

Computational statistical physics is about computing averages. Averages may be with respect to some statistical ensembles, which are prescribed by the physical context (for example, with respect to the canonical measure if the number of particles, the configuration space and the temperature are fixed, see (2) below). More complicated observables involve averages over trajectories, and this is the focus of this communication. The aim of this short note is to emphasize the crucial role played by *coarse-graining* in many efficient numerical techniques, and the importance of *metastability* to support the coarse-graining procedure.

To be more specific, let us consider the overdamped Langevin dynamics:

$$dX_t = -\nabla V(X_t)\, dt + \sqrt{2\beta^{-1}} dW_t \tag{1}$$

where $X_t \in \mathbb{R}^{3N}$ denotes the positions of N particles (think of a very large N), $V : \mathbb{R}^{3N} \to \mathbb{R}$ is a given potential, which to a set of positions $x \in \mathbb{R}^{3N}$ associates its energy $V(x)$, and $\beta^{-1} = k_B T$ is a constant proportional to the temperature.

This dynamics is prototypical of those considered in molecular dynamics. The difficulty when simulating (1) is that the typical timestep which is required to get a stable discretization is of the order of $10^{-15}s$, while the typical timescale over which interesting changes of conformations (namely macroscopically interesting modifications of the configurations X_t) are observed is of the order of $10^{-6}s$ (and even more in some cases). A natural question is then: how to get an equivalent dynamics, which could be obtained much more quickly than by a naive discretization of (1) ? One point we would like to emphasize here is that one really wants to get *correct trajectories*. This is not the same question as getting, for example, a sampling of the stationary measure for (1), which is indeed the canonical measure

$$\mu(dx) = Z^{-1} \exp(-\beta V(x))\, dx, \tag{2}$$

or a dynamics which would have only the correct evolution for the time marginals (namely the law of X_t at time t).

At this point, a natural idea is to try to reduce the dimension of the original problem, by only looking at some coarse-grained information, which would hopefully varies on a timescale which is much larger than $10^{-15}s$. Two ideas can be found in the literature. One may consider a function ξ defined on $\mathbb{R}^{3N}$ and with value in a *continuous low-dimensional space*, think for simplicity of the case of an angle in a molecule, in which case $\xi : \mathbb{R}^{3N} \to \mathbb{T}$ (where $\mathbb{T}$ is the one-dimensional torus). Another approach is to consider a function $\mathcal{S} : \mathbb{R}^{3N} \to \mathbb{N}$ with value in a *discrete space* which should be seen as a mapping from positions in $\mathbb{R}^{3N}$ to a state number in $\mathbb{N}$, these states constituting a partition of $\mathbb{R}^{3N}$. In both cases, the question is the following: is it possible to design (through a coarse-graining procedure) a good effective dynamics for $(\xi(X_t))_{t\geq 0}$, respectively for $(\mathcal{S}(X_t))_{t\geq 0}$? And, as mathematicians, we would even like to *quantify the error* introduced by the coarse-graining procedure. These coarse-graining techniques can then be used numerically to build efficient numerical techniques to integrate the dynamics (1) over macroscopically relevant timescales, and thus to circumvent the problems raised by metastability.

The take-home message of this note is that this is possible, and this requires to measure, in some sense, "the metastability of X_t along ξ, respectively along $\mathcal{S}$" (this is what is behind the assumptions (H1) and (H2) below). Let us make this more precise. For the first case (coarse-graining to a continuous state space dynamics), it is very natural to design an effective dynamics as follows (this can be seen as the so-called Mori-Zwanzig projection operator formalism). In a first step, by Itô's calculus, a non-closed dynamics on $\xi(X_t)$ can be written, namely:

$$d\xi(X_t) = \left(-\nabla V \cdot \nabla \xi + \beta^{-1}\Delta \xi\right)(X_t)\, dt + \sqrt{2\beta^{-1}}|\nabla \xi|(X_t) \frac{\nabla \xi}{|\nabla \xi|}(X_t) \cdot dW_t.$$

Then, one way to close the system is to introduce conditional expectations for the drift and the diffusion:

$$dz_t = b(z_t)\, dt + \sqrt{2\beta^{-1}}\sigma(z_t)\, dB_t$$

where B_t is a one-dimensional Brownian motion (one may think of $dB_t = \frac{\nabla\xi}{|\nabla\xi|}(X_t)\cdot dW_t$),

$$b(z) = \mathbb{E}_\mu\left(-\nabla V\cdot\nabla\xi + \beta^{-1}\Delta\xi(X)\,|\,\xi(X)=z\right)$$

and

$$\sigma^2(z) = \mathbb{E}_\mu\left(|\nabla\xi|^2(X)\,|\,\xi(X)=z\right).$$

What can then be shown is the following. If (H1) the Logarithmic Sobolev Inequality constant (or the Poincaré Inequality constant) of the conditional measures $\mu(\cdot|\xi(x)=z)$ are large, then the trajectories $(z_t)_{t\geq 0}$ are close to the trajectories $(\xi(X_t))_{t\geq 0}$. This can be shown on time-marginals, with error-estimates which are uniform in time [2] or through trajectorial estimates over finite time intervals, see [3]. We refer to these works for clearly formulated statements, with a complete set of assumptions. These assumptions (and in particular (H1)) are at the heart of many efficient numerical methods which have been proposed to circumvent some difficulties related to metastability for the computations of canonical averages and in particular free energy differences, see [5, 4].

For the second case, the idea is the following. For any trajectory $(X_t)_{t\geq 0}$ entering a new state, there are two possible situations: either the trajectory remains in the state for a very long time (let us call it τ_{corr}, following the notation of Art Voter [6]), or the trajectory leaves this new state before the time τ_{corr}. What we have shown in [1] is that, in the first situation (and if τ_{corr} is well chosen), the process is close to the *quasi-stationary distribution* associated to the current state, and therefore, conditionally to this state, the time it remains to go out is *exponentially distributed*, and *independent of the exit point* (and thus independent of the next visited state). These are the two fundamental properties required to build a discrete state space and continuous in time Markov process, in terms of state-to-state dynamics. It thus becomes clear that in this context, it is possible to build a coarse-grained Markovian dynamics if: (H2) the typical time it takes to leave a state is much larger than the time needed to reach the quasi-stationary distribution. This assumption is again at the heart of efficient numerical methods to generate very efficiently the dynamics $(\mathcal{S}(X_t))_{t\geq 0}$, and in particular the parallel replica algorithm, see [6]. We refer to [1] for a mathematical analysis and precise statements.

In both cases, the assumptions (H1) and (H2) can be seen as some mathematical formalizations of what is called metastability. Moreover, they can be used to quantify the degree of metastability of the process, typically in terms of Logarithmic Sobolev or Poincaré inequality constants, or spectral gaps of some Fokker-Planck operators. Designing efficient numerical techniques to estimate these constants would be a great step towards important improvements of currently used algorithms, and it is the subject of active research.

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Non-exit probability from a time-dependent region of a random walk among random conductances

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(joint work with Wolfgang König)

Random walk in random environment (RWRE) includes some of the most popular models in statistical physics and probability theory, contributing a lot towards the understanding of various phenomena such as mass transport or heat distribution in random media. The subfield of *random walk among random conductances (RWRC)* or, as many authors prefer to call it, *random conductance model (RCM)*, accounts for random spatial inhomogeneities in the diffusive dynamics, which seems in many respects more realistic than homogeneous diffusion modeled by a simple random walk. A considerable amount of research conducted on this topic has focused on deriving quenched invariance principles for the random walk, thus putting an emphasis on the asymptotic behaviour of the *end point* of the random walk. In contrast to that, the focus of our recent study has been the behaviour of *local times*, which means taking a closer look at the *whole path* of the walk. This talk addresses the simpler question of non-exit times from a region in the lattice growing with time.

Consider the lattice $\mathbb{Z}^d$ and assign to any edge (x, y) connecting two neighbouring sites $x \sim y$ a random weight $\omega_{x,y}$, subject to the symmetry condition $\omega_{x,y} = \omega_{y,x}$. Denote by $\mathcal{N}$ the canonical base of $\mathbb{Z}^d$, i.e., the set of neighbors of the origin with nonnegative entries. We assume that $(\omega_{x,x+e})_{x\in\mathbb{Z}^d, e\in\mathcal{N}}$ is a family of positive i.i.d. random variables and abbreviate $\omega(x, e) = \omega_{x,x+e}$. We intend to study the continuous-time random walk $(X_t)_{t\in[0,\infty)}$ in $\mathbb{Z}^d$ generated by the randomized Laplacian Δ^ω that acts on $l^2(\mathbb{Z}^d)$ as

$$\Delta^\omega f(x) := \sum_{y\in\mathbb{Z}^d\colon\, y\sim x} \omega_{x,y}(f(y) - f(x)), \qquad x \in \mathbb{Z}^d.$$

We focus on the annealed long-time behaviour of the random walk under the following assumptions on the lower tails of the conductance distribution. For any $x \sim y \in \mathbb{Z}^d$,

$$\operatorname{essinf}\{\omega_{x,y}\} = 0$$

and there exist positive parameters η and D such that, for any $x \sim y \in \mathbb{Z}^d$,

$$\log Prob(\omega_{x,y} \leq \varepsilon) \sim -D\varepsilon^{-\eta} \quad \text{as } \varepsilon \searrow 0.$$

Here, *Prob* refers to the probability with respect to ω. Let us write $\langle\cdot\rangle$ for the expectation with respect to ω and $\mathbb{E}_0^\omega$ for the expectation with respect to the random walk starting at the origin. With $B \subset \mathbb{R}^d$ some finite, convex and open set containing the origin and α_t some sufficiently regular scaling function with $1 \ll \alpha_t \ll t^{\frac{1}{d+2}}$, the asymptotic behaviour of the annealed non-exit probabilities

$$\begin{aligned} p_t(B) &= \langle \mathbb{E}_0^\omega(X_{[0,t]} \subset B)\rangle \qquad \text{and} \\ P_t(B) &= \langle \mathbb{E}_0^\omega(X_{[0,t]} \subset \alpha_t B)\rangle \end{aligned}$$

is determined by certain variational problems the solvability of which depends on the parameter η. Consider

$$\chi_d(B) = \inf\Big\{ \sum_{e\in\mathcal{N}, z\in B\cap\mathbb{Z}^d} |f(z+e)-f(z)|^{\frac{2\eta}{1+\eta}} : f \in l^2(\mathbb{Z}^d),\, \mathrm{supp} f \subset B,\, \|f\|_2 = 1\Big\}. \tag{1}$$

and

$$\chi_c(B) = \inf\Big\{ \sum_{e\in\mathcal{N}} \int_B |\partial_e f(y)|^{\frac{2\eta}{1+\eta}}\, \mathrm{d}y :\ f \in H_0^1(B),\, \|f\|_2 = 1\Big\}. \tag{2}$$

By dint of discrete and continuous Sobolev inequalities and other compactness criteria, we have

i) $\chi_d(B) > 0$.
ii) $\chi_c(B) > 0$ if $\eta \geq d/2$.
iii) $\chi_c(B) = 0$ and $\chi_d(\mathbb{R}^d) > 0$ if $\eta < d/2$.

In [3], it was shown as a corollary to the main result that

$$\log p_t(B) \sim -K_{\eta,D}\, t^{\frac{\eta}{\eta+1}} \chi_d(B) \tag{3}$$

where $K_{\eta,D} = \big(1+1/\eta\big)(D\eta)^{1/(1+\eta)}$. This behaviour is due to a combined "effort" of the conductances and the random walk to stay in the finite region. More precisely, the main contribution to the non-exit probability comes from the time-dependent event

$$\{\beta_t\omega(z,e) \approx \varphi(z,e) \text{ for all } z \in B\cap\mathbb{Z}^d, e \in \mathcal{N}\}$$

with a well-balanced scale β_t and an optimally chosen function $\varphi : B\cap\mathbb{Z}^d \times \mathcal{N} \to (0,\infty)$. Restricted to this event, the annealed non-exit probability decays exponentially with scale $t\beta_t^{-1}$ by the Donsker-Varadhan-Gärtner Large Deviations principle (compare [1],[2]). The optimal scale β_t is found by balancing this scale with the probabilistic cost of the untypical conductance behaviour and the optimal

rate arises when choosing φ in an optimal way. By the same approach, one could on a heuristic level argue that

$$\log P_t(B) \sim -K_{\eta,D}\, t^{\frac{\eta}{1+\eta}}\, \alpha_t^{\frac{d-2\eta}{1+\eta}}\, \chi_c(B).$$

However, in the case $\eta < d/2$ which corresponds to a strong tendency of the conductances to attain very small values, we have $\chi_c(B) = 0$. Here, sequences of functions approximating the infimum in (2) have the tendency to mount up at the origin. As the minimisers of (2), if they exist, admit an interpretation as typical rescaled occupation time profiles of the random walk, this gives rise to the underlying picture of the random walk refusing to spread over the area $\alpha_t B$ due to the *high* probabilistic cost of having small conductances on that whole area. On the contrary, the random walk stays in a much smaller region (corresponding to huge peaks of the rescaled occupation time profile at the origin), which is supported by the relatively *low* probabilistic cost of having small conductances in just that small region. These considerations lead us to the conjecture that

$$\log P_t(B) \sim \begin{cases} -K_{\eta,D}\, t^{\frac{\eta}{1+\eta}}\, \alpha_t^{\frac{d-2\eta}{1+\eta}}\, \chi_c(B) & \text{if } \eta \geq d/2, \\ -K_{\eta,D}\, t^{\frac{\eta}{1+\eta}}\, \chi_d(\mathbb{R}^d) & \text{if } \eta < d/2. \end{cases} \tag{4}$$

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Thermalization of rate-independent processes by entropic regularization

Timothy Sullivan

(joint work with Marisol Koslowski, Florian Theil and Michael Ortiz)

Many evolutionary problems of interest take the form of a *gradient descent*: a trajectory that is the steepest descent in a space $\mathcal{Q}$ of an energy functional E with respect to some dissipation functional Ψ. The state space $\mathcal{Q}$ is, in general, a metric space that may lack any linear or differentiable structure [1]. Typically, the dissipation potential Ψ is assumed to have superlinear growth at infinity; if instead Ψ is homogeneous of degree 1, then the resulting evolutionary system is *rate-independent* (or *quasi-static*) in the sense that the solution operator commutes with strictly increasing reparametrizations of time. Rate-independent processes model hysteretic phenomena such as plasticity and phase transformations in elastic solids, electromagnetism, dry friction on surfaces, and pinning problems

in superconductivity; such models are limiting models in the limit of vanishing inertia, relaxation times, and thermal effects [5].

We consider a model for the influence of a heat bath upon a rate-independent evolution that takes values in a (finite-dimensional, smooth) Riemannian manifold $(\mathcal{Q}, g)$ over an interval of time $[0, T]$. The energetic potential is $E\colon [0,T] \times \mathcal{Q} \to \mathbb{R}$; the dissipation potential is $\Psi\colon [0,T] \times \mathrm{T}\mathcal{Q} \to [0, +\infty)$ and is is assumed to be continuous, convex, non-degenerate and homogeneous of degree 1 on each tangent space — *i.e.* Ψ defines a time-dependent Finsler metric on $\mathcal{Q}$.

Given $h > 0$ and discrete times $(t_i := ih)_{i=0}^{T/h}$, the incremental variational formulation of the rate-independent problem is to find states $(z_i)_{i=0}^{T/h} \subseteq \mathcal{Q}$ such that each z_{i+1} minimizes

$$W(z_i, z_{i+1}) := E(t_{i+1}, z_{i+1}) - E(t_i, z_i) + h\Psi\big(\mathrm{Log}_{z_i} z_{i+1}/h\big), \tag{1}$$

where Log_z denotes the inverse of the exponential map Exp_z from $\mathrm{T}_z\mathcal{Q}$ into $\mathcal{Q}$. The continuous-time rate-independent process $z\colon [0,T] \to \mathcal{Q}$ is the limit as $h \to 0$ of the interpolants of the solutions to (1), and is the Ψ-gradient descent in E:

$$\mathrm{D}\Psi(t, z(t), \dot{z}(t)) \ni -\mathrm{D}E(t, z(t)).$$

We posit a Markov chain model for the effect of a heat bath working with constant power $\theta > 0$ (*i.e.* the heat bath supplies energy proportional to θh over each subinterval $[t_i, t_{i+1}]$): we consider the $\mathcal{Q}$-valued Markov chain Z^h with transition probabilities having density

$$\rho(z_{i+1}|z_i) \propto \exp\big(-W(z_i, z_{i+1})/\theta h\big) \tag{2}$$

with respect to the Riemannian volume measure $\mathrm{dVol}_{(\mathcal{Q},g)}$. This density has the variational characterization that it minimizes

$$\int_{\mathcal{Q}} \big(W(z_i, \cdot)\rho(\cdot|z_i) + \theta h\, \rho(\cdot|z_i) \log \rho(\cdot|z_i)\big)\, \mathrm{dVol}_{(\mathcal{Q},g)},$$

and so the Markov chain model can be seen as a competition between the energetic considerations (1) of the original gradient descent and entropic considerations. The natural objective is to identify the continuous-time limit process of Z^h as $h \to 0$.

If Ψ is homogeneous of degree 2, then the scheme (2) corresponds to the addition of Itō noise to generate a stochastic gradient descent in E as in [4]. Our main result is that when Ψ is homogeneous of degree one, although Z^h is a stochastic process with non-trivial distribution for each $h > 0$, the limit process as $h \to 0$ is a deterministic rate-*dependent* process. Furthermore, the limit process is, up to sign, a gradient descent in E with respect to a new, nonlinear, dissipation potential $\widetilde{\Psi}\colon [0,T] \times \mathrm{T}\mathcal{Q} \to [0, +\infty)$.

More precisely, let $\widetilde{\Psi}$ denote the *Cramer transform* of Ψ, defined by

$$\widetilde{\Psi}^\star(t, x, \ell) := \log \int_{\mathrm{T}_x\mathcal{Q}} \exp\big(-(\langle \ell, v\rangle + \Psi(t, x, v))\big)\, \mathrm{d}v \qquad \text{for } \ell \in \mathrm{T}_x^*\mathcal{Q}, \tag{3}$$

$$\widetilde{\Psi}(t, x, v) := \sup\big\{\langle \ell, v\rangle - \widetilde{\Psi}^\star(t, x, \ell) \,\big|\, \ell \in \mathrm{T}_x^*\mathcal{Q}\big\} \qquad \text{for } v \in \mathrm{T}_x\mathcal{Q}. \tag{4}$$

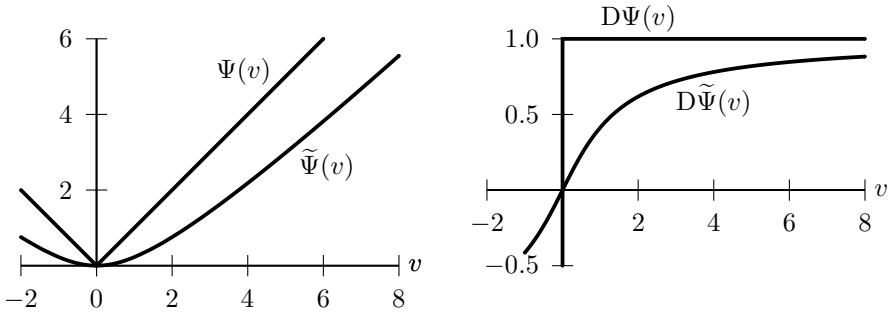

FIGURE 1. Comparison of the dissipation potential $\Psi := |\cdot|$ on $\mathbb{R}$ and its Cramer transform $\widetilde{\Psi}$ as defined by (3)–(4), and their (sub-)derivatives. In this case, $\widetilde{\Psi}^\star(\ell) = -\log(1-\ell^2)$; $\mathrm{D}\widetilde{\Psi}$ can be calculated using the relation $\ell \in \mathrm{D}\widetilde{\Psi}(x) \iff x \in \mathrm{D}\widetilde{\Psi}^\star(\ell)$.

The Cramer transform $\widetilde{\Psi}$ is a strict convexification and smoothing-out of Ψ. It exhibits quadratic behaviour near the origin (slow evolutionary rates) and linear growth at infinity (fast evolutionary rates); see Figure 1.

The limit process of Z^h as $h \to 0$ is the solution $y\colon [0,T] \to \mathcal{Q}$ of

$$\mathrm{D}\widetilde{\Psi}\big(t, y(t), -\dot{y}(t)/\theta\big) = \mathrm{D}E(t, y(t)), \tag{5}$$

and, under suitable conditions, Z^h converges to y in probability as $h \to 0$, *i.e.*

$$\lim_{h\to 0} \mathbb{P}\left[\sup_{t\in[0,T]} d_{(\mathcal{Q},g)}\big(Z^h(t), y(t)\big) \geq \delta\right] = 0 \text{ for every } \delta > 0. \tag{6}$$

The intuition behind this result is that, to a first approximation,

$$\mathbb{E}\big[\mathrm{Log}_{z_i} Z^h_{i+1} \big| Z^h_i = z_i\big] \approx -\theta h\, \mathrm{D}\widetilde{\Psi}^\star\big(t_i, z_i, \mathrm{D}E(t_i, z_i)\big),$$
$$\mathbb{V}\big[\mathrm{Log}_{z_i} Z^h_{i+1} \big| Z^h_i = z_i\big] \approx (\theta h)^2\, \mathrm{D}^2\widetilde{\Psi}^\star\big(t_i, z_i, \mathrm{D}E(t_i, z_i)\big),$$

and so the variance is expected to be negligible in the limit as $h \to 0$, leaving only the mean flow (5). The principal condition necessary to ensure the convergence (6) is that the curvature of $(\mathcal{Q}, g)$ and the vector field $f(t,x) := -\mathrm{D}\widetilde{\Psi}^\star\big(t, x, \mathrm{D}E(t,x)\big)$ be such that geodesics starting at (t,x) and (t,x') near to the trajectory of y with initial velocities given by $f(t,x)$ and $f(t,x')$ do not diverge too quickly. When $\mathcal{Q} = \mathbb{R}^n$ with its usual metric, this corresponds to the requirement that f be a monotone vector field [7], at least near the trajectory of y.

As shown in [6], this result predicts rheological power laws such as the Andrade creep law for soft metals. Andrade [2, 3] observed that soft metals exposed to constant subcritical applied stress at room temperature exhibited strain $\sim t^{1/3}$ for short time, and $\sim t$ in long time. Under the assumption of linear strain hardening and constant applied load — *i.e.* the dissipation potential $\Psi(t,x,v) = x|v|$ on $\mathcal{Q} = (0, +\infty)$ and energetic potential $E(t,x) = -\ell x$ with $|\ell| < 1$ — Andrade's law appears naturally, since in this setting solutions to (5) do indeed grow $\sim t^{1/3}$.

This example justifies posing the problem on a manifold with state-dependent dissipation functional instead of the simpler setting of $\mathbb{R}^n$ with a state-independent dissipation functional: the Andrade creep law would not be obtained in the simpler setting. Furthermore, some rate-independent problems on $\mathbb{R}^n$ have a dissipation functional Ψ that is 0 or $+\infty$ in some directions; restricting attention to a submanifold of $\mathbb{R}^n$ on which Ψ is well-behaved can circumvent these difficulties.

It would be of interest to extend the above results to evolutions in spaces without a locally linear, smooth, or finite-dimensional structure, as in [1].

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On the speed of Random Walks among Random Conductances

Michele Salvi

(joint work with Noam Berger)

Random Walks among Random Conductances (RWRC), also known in the literature as *Random Conductance Model (RCM)*, is a particular kind of *Random Walks in Random Environment (RWRE)*. Consider, for simplicity, the grid $\mathbb{Z}^d$ and the set E^d of its unoriented edges $\{x, y\}$, with $x \sim y \in \mathbb{Z}^d$ nearest neighbours. Consider the measure space $\Omega_d = [0, \infty)^{E^d}$. For a given $\omega \in \Omega_d$ and $z \in \mathbb{Z}^d$ we define P_z^ω to be the law of a Markov chain on $\left(\mathbb{Z}^d\right)^{\mathbb{N}}$ with $P_z^\omega(X_0 = z) = 1$ and

$$P_z^\omega(X_{n+1} = y | X_n = x) = \frac{\omega(x, y)}{\sum_{w \sim x} \omega(x, w)}, \qquad \forall x, y \in \mathbb{Z}^d,\, x \sim y,$$

where $\omega(x, y)$ is the value of ω on the bond $\{x, y\}$, called its *conductance*.

The community is currently putting a lot of effort in proving functional-central-limit kind of statements, that is the convergence to some diffusion of the space-time rescaled process, or other fine properties of the walk in the case of random ergodic conductances. Taking one step back, we focused on the incomplete picture of the problem of the *Law of Large Numbers*.

Call $\lim_{n\to\infty} \frac{X_n}{n}$ the *limiting speed*, or just speed, of the process. For an event A, the annealed law is $\mathbb{P}(A) = \int_{\omega\in\Omega_d} P_0^\omega(A)\,\mathrm{d}Q(\omega)$, where $Q \in \mathcal{M}_1(\Omega_d)$ is the given law from which we sample our conductances.

It is well known that the cases of conductances i.i.d. or bounded from above have almost surely zero annealed speed. Let now $Q \in \mathcal{M}_1(\Omega_2)$ be invariant and ergodic w.r.t. the group of spatial shifts in $\mathbb{Z}^2$. Our question is: are there sufficient conditions on the moment of the conductances for the speed to be equal to zero?

It turns out that if the expectation $E^Q[\log^\alpha \omega(x,y)]$ is finite for some $\alpha > 1$, then the random walk has almost surely speed zero. This can be easily proven via the classical Varopulos-Carne heat kernel estimates (see, e.g. [2]).

This condition is sharp in the following sense: we can provide examples of RWRC for which the limiting speed is non-zero and $E^Q[\log^\alpha \omega(x,y)] < \infty$ for α arbitraily close to 1 from below. Exploiting the construction of a random spanning tree provided in the article [1], we show in fact examples for which the resulting process does not have any speed, meaning that X_n/n does not admit limit almost surely. Modifying the aforementioned construction, we can finally provide environment laws which guarantee the RWRC to have almost surely positive speed.

This results can be also generalized to higher dimentions.

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Random walks in random environment on a strip

Jan Nagel

(joint work with Nina Gantert)

For a random walk in random environment (RWRE) in dimension higher than one, there is no known characterisation of recurrence or transience. We consider this question in the case of a random walk on the strip $\mathbb{Z} \times \{1, \dots, m\}$. In this case, Bolthausen and Goldsheid [1] found criteria for recurrence and transience in term of Lyapunov exponents. We are interested in explicit criteria in the situation where the transition probabilities in horizontal direction are random and i.i.d. for different columns and transition probabilities in vertical direction are fixed. This model can be interpreted as a combination of m different one-dimensional RWRE. We investigate the question whether recurrence depends on the probability γ of vertical movements.

Even in this particular case, the random walk shows an interesting behaviour: we may have that all random walks restricted to a single row are transient to $+\infty$, but for any $\gamma \in (0,1)$, the random walk on the strip is transient to $-\infty$.

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Wasserstein gradient flows from large deviations of thermodynamic limits

Vaios Laschos

(joint work with Manh Hong Duong and Michiel Renger)

We are concerned with the Fokker-Planck equation $\frac{\partial \rho}{\partial t} = \Delta\rho + \nabla \cdot (\rho \nabla \Psi)$, for subquadratic potentials Ψ and $t \in [o, \tau]$. We study the equation as the hydrodynamic limit of a stochastic particle system and try to highlight a link with the Wasserstein gradient flow of the free energy $\mathcal{F}(\rho) = \int_{R^d} (\Psi(x) + \log \rho(x))\rho(x)dx$. For "good" initial data ρ_0, we describe the curves for which the rate functional

$$\tilde{J}_\tau(\rho(\cdot)) = \frac{1}{4\tau} \int_0^1 \left\| \frac{\partial \rho_t}{\partial t} - \tau(\Delta \rho_t + \nabla \cdot (\rho_t \nabla \Psi)) \right\|^2_{-1,\rho_t} dt \tag{1}$$

that characterizes the large deviations from the hydrodynamic limit, has a finite value. For these curves, we rewrite the above functional in a way that the free energy and its gradient appear explicitly

$$\tilde{J}_\tau(\rho(\cdot)) = \frac{1}{4\tau} \int_0^1 \left\| \frac{\partial \rho_t}{\partial t} \right\|^2_{-1,\rho_t} dt + \frac{\tau}{4} \int_0^1 \|\nabla \mathcal{F}(\rho)\|^2_{-1,\rho_t} \, dt + \frac{1}{2}\mathcal{F}(\rho_1) - \frac{1}{2}\mathcal{F}(\rho_0).$$

Next we use this formulation via the contraction principle to prove that the time discreet rate functional

$$J_\tau(\rho|\rho_0) = \inf \left\{ \mathcal{H}(\gamma|\rho_0 \otimes p_\tau) : \gamma \in \Pi(\rho_0, \rho) \right\}$$

is asymptotically equivalent in the Γ-convergence sense to the functional derived from the Wasserstein gradient discretization scheme

$$\frac{1}{2}\mathcal{F}(\rho) - \frac{1}{2}\mathcal{F}(\rho_0) + \frac{1}{4\tau} W_2^2(\rho_0, \rho).$$

This extends the results in [2, 1, 3] to all probability measures in the real line with finite second moment.

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Gradient flows driven by a non-smooth repulsive interaction potential

Giovanni Bonaschi
(joint work with Giuseppe Savaré)

The description of a great variety of phenomena, from crowd dynamics to chemotaxis, is achieved via the following non-local interaction equation

$$\frac{\partial \mu}{\partial t} = \nabla \cdot (\mu(\nabla W * \mu)) \qquad x \in \mathbb{R}^d \ , \ t > 0.$$

We search for weak measure solutions, and it has been shown in [1] that the equation can be nicely restated as a Wasserstein Gradient Flow of the interaction functional below:

$$\mathcal{W}[\mu] = \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} W(x-y) d\mu(x) d\mu(y).$$

The existence and uniqueness of a gradient flow solution requires certain hypothesis on the interaction potential W (see [1, 2]): $W(x) = W(-x)$, $W \in C^1(\mathbb{R}^d \setminus \{0\})$, W has at most a quadratic growth at infinity and, of crucial importance, W is λ-convex (i.e. $\exists \lambda < 0$ s.t. $W(x) - \lambda |x|^2$ is convex).
We study the problem when the λ-convexity is lost (other works exploring the same direction are [3, 4, 5, 6, 7, 8]), more precisely we ask for a weaker condition:

$$\exists \lambda, \lambda' < 0 \text{ such that } W(x) - \lambda' |x|^2 - \lambda |x| \text{ is convex.}$$

In fact we allow the potential to present a concave cusp in the origin. With this choice we can represent a strong repulsive behaviour at short distances. We can decompose a general W satisfying our weaker hypothesis in a sum: $\bar{W} - c|x|$ with $\bar{W}$ with all the regularity needed and with c constant. Because of this we limit our analysis to the case $W = |x|$ without loss of generality (the constant is equal to one for simplicity). Following the idea of [2] we analyze the ODE system that give us trial solution in case of concentrated mass and in the $1d$ case we can use the monotone rearrangement.
The analysis of the ODE system show us that a solution exist for the starting equation, but there are infinite of them. The idea is that the gradient flow formulation can be a way to make a selection in the set of all the solutions. We prove existence and uniqueness of solution for the $1d$ problem. Simple examples show that the gradient flow solution select a diffusive evolution. It means, thinking at the time reversal, that after the aggregation of solutions there is a loss of information, it is impossible to determine the starting probability density that generated the aggregation, only one is selected among all the other. An explicit formula has been obtained for a general potential and it turns out that a Dirac delta cannot remain a Dirac delta at every time $t > 0$.

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Stabilization due to additive noise

Dirk Blömker

Stabilization due to noise is a well-known phenomenon, and there are numerous publications over the last decades. But most examples are for multiplicative noise only. Stabilization can arise somewhat artificially by adding Itô-noise, due to the Itô-Stratonovich correction, as only multiplicative Stratonovich-noise is neutral for the linear stability. In other cases stabilization arises due to averaging over stable and unstable directions. A celebrated example is Kapiza's problem of the inverted pendulum [13]. This averaging is also effective in case of deterministic rotation of the system [10]. But there are very few examples due to additive noise. Very nice is the blow-up through a small tube [15].

We consider two very simple examples of stochastic partial differential equations (SPDEs) close to bifurcation. Using the natural separation of time scales, one derives effective stochastic differential equations (SDEs) for the amplitudes of the dominating pattern. Due to averaging, the noise not acting directly on the dominant pattern may appear as a stabilizing deterministic correction to the SDEs.

Swift-Hohenberg equation. In a series of papers [11, 12], it was numerically and formally (using a center-manifold argument) justified that additive noise is capable of removing patterns in the one-dimensional Swift-Hohenberg equation. See also [9]. The Swift-Hohenberg equation is an SPDE given by

$$\partial_t u = -(1+\partial_x^2)^2 u + \nu\epsilon^2 u - u^3 + \sigma\epsilon\partial_t\beta \tag{SH}$$

subject to periodic boundary conditions on $[0, 2\pi]$ and β being a real-valued Brownian motion. The constants σ and ν measure the noise strength and the distance

from bifurcation, respectively. The eigenfunctions of the differential operator are $\sin(kx)$ and $\cos(kx)$, $k \in \mathbb{Z}$. The kernel $\mathrm{span}\{\sin, \cos\}$ is the space of the dominant pattern. Using the Ansatz

$$u(t,x) = \epsilon A(\epsilon^2 t)\mathrm{e}^{ix} + c.c. + \epsilon\sigma Z(t) + \mathcal{O}(\epsilon^2) \ ,$$

with a fast Ornstein-Uhlenbeck (OU) process $Z(t) = \int_0^t e^{-(t-\tau)} d\beta(\tau)$ and complex-valued amplitude A, we obtain the following amplitude equation [6]:

$$\text{(A)} \qquad \partial_T A = (\nu - \tfrac{3}{2}\sigma^2)A - 3A|A|^2 \ .$$

It is interesting that the amplitude equation for the dominant behavior is deterministic, and noise leads to a stabilizing deterministic correction. For a precise statement and proof of the approximation result see [6], which treats a more general situation. Numerical approximation [9] shows that any moment of the uniform in space and time error grows logarithmically with the time-interval, while moments of the error for a fixed time seem to stay small for very long times.

Averaging with error bounds. In formal calculations for the derivation of the amplitude equation, the additional constant terms arise from square of noise in $3A\sigma^2(\epsilon\partial_T\tilde{\beta})^2$, where $\tilde{\beta}(T) = \epsilon\beta(T\epsilon^{-2})$ is a rescaled Brownian motion on the slow time-scale $T = \epsilon^2 t$. In the proofs, using the mild formulation (i.e., variation of constants), we consider the fast OU-process

$$Z(T\epsilon^{-2}) = Z_\epsilon(T) = \epsilon^{-1}\int_0^T e^{-(T-s)\epsilon^{-2}} d\tilde{\beta}(s) \approx \epsilon\partial_T\tilde{\beta}(T) \ .$$

Crucial for the derivation of averaging with explicit error bounds is the following Lemma based on Itô's formula:

Lemma [4, 7] *Let X be a stochastic process with bounded initial condition and differentials, i.e. $dX = \mathcal{O}(\epsilon^{-r})dt + \mathcal{O}(\epsilon^{-r})d\tilde{\beta}$ and $X(0) = \mathcal{O}(\epsilon^{-r})$ for some $r > 0$. Then*

$$\int_0^T X(s)Z_\epsilon(s)^2 ds = \tfrac{1}{2}\int_0^T X(s)ds + \mathcal{O}(\epsilon^{1-2r}) \ .$$

Similar results hold true for other even powers of Z_ϵ. For odd powers we have

$$\int_0^T X(s)Z_\epsilon(s)ds = \mathcal{O}(\epsilon^{1-r}) \ , \qquad \int_0^T X(s)Z_\epsilon(s)^3 ds = \mathcal{O}(\epsilon^{1-3r}) \ , \qquad \cdots$$

Note that $X = \mathcal{O}(f_\epsilon)$, if for all $p > 1$ and $T > 0$ there is a $C > 0$ such that

$$\mathbb{E}\sup_{s\in[0,T]}|X(s)|^p \le C{f_\epsilon}^p \ .$$

Burgers type equation. Stabilization effects were observed numerically in [1, 14] for an equation of the following type;

$$\text{(B)} \qquad \partial_t u = -(1+\partial_x^2)u + \nu\epsilon^2 u + \tfrac{1}{2}\partial_x u^2 + \sigma\epsilon\partial_t\beta\sin(2\cdot)$$

subject to Dirichlet boundary conditions on $[0,\pi]$ with dominant space $\mathrm{span}\{\sin\}$. The highly degenerate noise acts only on the 2^{nd} mode by β. Consider:

$$u(t,x) = \epsilon a(\epsilon^2 t)\sin(x) + \epsilon\sigma Z(t)\sin(2x) + \mathcal{O}(\epsilon^2)$$

with fast OU-process $Z(t) = \int_0^t e^{-3(t-\tau)} d\beta(\tau)$. This is rigorously justified by a-priori estimates. In [4] we obtain the following amplitude equation:

$$da = (\nu - \tfrac{\sigma^2}{88})a\, dT - \tfrac{1}{12}a^3 dT + \tfrac{\sigma}{6} a \circ d\tilde{\beta} \tag{A2}$$

in Stratonovich sense, with rescaled Brownian motion $\tilde{\beta}(T) = \epsilon\beta(\epsilon^{-2}T)$. Obviously, 0 is stabilized for $\nu \in (0, \sigma^2/88)$. For a precise statement of the approximation result and its proof in a significantly generalized situation see [4]. Numerical justification in [9] verified the validity of the approximation for large times and moderate or even large ϵ.

Outlook – Open problems. We comment on a series of related results, generalizations and open problems. Interesting questions in regularity and scaling arise for example for Levy noise [5].

Averaging of martingals of the type $\int_0^T X Z_\epsilon^q d\beta$ is necessary for (B) with high-dimensional noise or for higher order corrections for (SH). The averaging is well known, but for error estimates in [4] we are based on Levy's characterization theorem, restricting the result to one-dimensional dominant modes.

Modulated patterns arise if the underlying domain is large or unbounded. Here we need to approximate by a modulated wave of the type $A(\epsilon^2 t, \epsilon x)e^{ix} + c.c.$, where A solves a SPDE of Ginzburg-Landau type. See [4, 8]. The truly unbounded space with space-time white noise is still open. Solutions seem to be both spatially unbounded and not sufficiently regular for the tools available.

The results presented are limited to long transient time-scales. For the approximation of long-time behavior in terms of invariant measures for (SH) see [2].

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Homogenization of random parabolic operators. Diffusion approximation

Andrey L. Piatnitski
(joint work with Marina Kleptsyna and Alexandre Popier)

The talk focuses on homogenization problem for divergence form second order parabolic operators whose coefficients are rapidly oscillating functions of both spatial and temporal variables. The corresponding Cauchy problem takes the form

$$\begin{aligned} &\frac{\partial u^\varepsilon}{\partial t} = \operatorname{div}\Big(a\Big(\frac{x}{\varepsilon}, \frac{t}{\varepsilon^\alpha}\Big)\nabla u^\varepsilon)), \qquad (x,t) \in \mathbb{R}^d \times (0,T) \\ &u^\varepsilon(x,0) = g(x), \qquad u^\varepsilon\big|_{\partial G} = 0, \end{aligned} \tag{1}$$

with $g(x) \in L^2(\mathbb{R}^d)$. We assume that the coefficients of $a(z,s)$ are periodic functions of spatial variables while their dependence of time is random stationary ergodic, $\alpha > 0$. Moreover, the matrix $a(z,s)$ is real symmetric, uniformly bounded and positive definite.

It was proved in [1], [2] that the solutions of the original problem converges almost surely to a deterministic limit, the limit function being a solution of homogenized equation with constant coefficients:

$$\frac{\partial u^0}{\partial t} = \operatorname{div}(a^{\text{eff}}\nabla u^0), \qquad u^0(x,0) = g(x), \tag{2}$$

The question of interest is the asymptotic behaviour of the normalized difference of the original and homogenized solutions.

It turns out that the limits behaviour of the said normalize difference depends crucially on whether $\alpha < 2$, or $\alpha = 2$, or $\alpha > 2$. In the talk we mostly dwell on the the self-similar case $\alpha = 2$.

In order to formulate the diffusion approximation result we need an auxiliary function, so-called corrector.

Lemma (see [3]). *The equation*

$$\partial_s \chi(z,s) = \operatorname{div}_z\big(a(z,s)[\nabla_z \chi(z,s) + \mathbf{I}]\big)$$

has a stationary in s and periodic in z solution. The solution is unique up to an additive (random) constant.

We now consider the expressions

$$V^\varepsilon := \frac{u^\varepsilon - u^0}{\varepsilon} - \chi\Big(\frac{x}{\varepsilon}, \frac{t}{\varepsilon^2}\Big)\nabla u^0.$$

We also introduce the strong mixing coefficient. First we define the following σ-algebras:

$$\mathcal{F}_{\le t} = \sigma\{a(\cdot, s) \,:\, s \le t\}$$

$$\mathcal{F}_{\ge t} = \sigma\{a(\cdot, s) \,:\, s \ge t\}$$

Definition (Strong mixing coefficient)**.**

$$\beta(r) = \sup_{\substack{A\in\mathcal{F}_{\le 0},\\ B\in\mathcal{F}_{\ge r}}} |\mathbb{P}(A\cap B) - \mathbb{P}(A)\mathbb{P}(B)|.$$

Our main result is

Theorem 1. *Let $\alpha = 2$, and suppose $g \in C^1(\mathbb{R}^d)$. Assume, moreover, that the function $\beta(r)$ decays fast enough so that*

$$\int_0^\infty \sqrt{\beta(r)}\, dr < \infty.$$

Then the normalized difference

$$V^\varepsilon(x,t) = \frac{1}{\varepsilon}\Big\{u^\varepsilon(x,t) - u^0(x,t) - \varepsilon\chi\Big(\frac{x}{\varepsilon}, \frac{t}{\varepsilon^2}\Big)\nabla u^0(x,t)\Big\}$$

converges in law in $L^2((0,T)\times\mathbb{R}^d)$ to a solution of the following SPDE with constant coefficients:

$$dV = [a^{\text{eff}}\frac{\partial^2}{\partial x^2}V + \mu\frac{\partial^3}{\partial x^3}u^0]\, dt + \Lambda\frac{\partial^2}{\partial x^2}u^0\, dW_t, \qquad V(0) = 0.$$

The tensors $\mu = \mu_{ijk}$ and $\Lambda = \Lambda_{ij}^{kl}$ can be found in terms of solutions of appropriate auxiliary cell problems.

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Dynamics of Crystal Growth with Corner Regularization

Nung Kwan Yip
(joint work with Fang Wan)

We investigate a dynamic model of a two dimensional crystal growth described by a forward-backward parabolic equation. The ill-posed region of the equation is handled by incorporating the motion of corners on the surface. We analyze a fourth order regularized version of this equation and show that the dynamical behavior of the regularized corner can be described by a travelling wave solution. The speed of the wave is found by rigorous asymptotic analysis. The interaction between multiple corners and the behavior of wrinkled surfaces (described by pulsating waves) are also investigated by asymptotic analysis and numerical simulation.

Introduction. The crystal growth problem, in its simplest form originates from the following anisotropic isoperimetric problem:

$$\min\left\{E(\partial\Omega) := \int_{\partial\Omega} \gamma(\theta)\, ds \ \text{ with } \text{Area}(\Omega) = 1\right\} \tag{1}$$

where $\gamma : S^1 \longrightarrow R_+$ is the *surface energy integrand*, θ is the angle of the outward normal $\hat{n}$ to $\partial\Omega$ and s is the arc-length parameter. (Note that in two dimensions, the crystal surface $\partial\Omega$ is a curve.) The solution is given by the classical Wulff construction:

$$W = \left\{x : x \cdot \hat{\theta} \le \gamma(\theta), \ \text{ for all } \theta\right\} \quad (\hat{\theta} \text{ is the unit vector in the direction of } \theta).$$

Formation of *corners* and *facets* in the Wulff shape are due to the *extreme anisotropy* and *cusps* in the γ-plot. See [1, 4] for an explanation of the relevant concepts.

The Wulff shape can also be described analytically by the following Euler-Lagrange equation:

$$(\gamma(\theta) + \gamma''(\theta))\kappa = \mu \qquad \left(\kappa = \frac{\partial\theta}{\partial s}\right), \tag{2}$$

where κ is the curvature and μ is the Lagrange multiplier for the area constraint in (1). Denoting $\Gamma(\theta) = \gamma(\theta) + \gamma''(\theta)$, corner arises when the surface normal $\hat{n}$ tries to avoid the unstable directions related to the range of angles on which Γ is negative. Another interpretation is in terms of the Frank diagram: $\theta \longrightarrow \frac{1}{\gamma(\theta)}$. It can be shown that the Frank diagram is *convex* at θ if and only if $\Gamma(\theta)$ is *positive*. The limiting directions θ_c^+ and θ_c^- of the two sides of a corner can be calculated explicitly by looking at the places where the Maxwell line touches the Frank diagram. Essentially, directions in the range (θ_c^-, θ_c^+) do not appear due to their non-energy minimizing property.

In terms of dynamics, we consider the *negative L^2-gradient flow* of the energy E, leading to the following *anisotropic motion by mean curvature*:

$$V_n = \Gamma(\theta)\kappa \qquad (V_n \text{ is the normal velocity}). \tag{3}$$

Due to the combined presence of the positivity and negativity of Γ, the above motion law is a forward-backward parabolic equation. A method to handle this is

again to introduce corners whose locations now can evolve in time. See [2] and [6] for a precise description and analysis of this approach using classical and viscosity solution methods. The goal of this work is to understand dynamics (3) in the presence of corners from the point of view of singular perturbations.

Corner Regularization. The work [8] considers the following regularized version of the energy E in (1):

$$E_\epsilon(\partial\Omega) := \int_{\partial\Omega} \gamma(\theta) + \frac{1}{2}\epsilon^2\kappa^2(\theta)\, ds. \tag{4}$$

Then the Euler-Lagrange equation (2) is modified to

$$\Gamma(\theta)\kappa - \epsilon^2\left(\frac{\partial^2\kappa}{\partial s^2} + \frac{1}{2}\kappa^3\right) = \mu. \tag{5}$$

The above model also appears in [7, 3, 5]. The corner in the non-regularized version is smoothened at length-scale ϵ. The above equation can be solved quite explicitly. The limiting corner angles $\theta_c^\pm$ can also be recovered from the solution procedure.

The regularized version of the motion law (3) now becomes:

$$V_n = \Gamma(\theta)\kappa - \epsilon^2\left(\kappa_{ss} + \frac{1}{2}\kappa^3\right). \tag{6}$$

For the ease of understanding and analysis, we consider the following small slope approximation of the above equation using a graph representation of $\partial\Omega$:

$$u_t = \widetilde{\Gamma}(u_x)u_{xx} - \epsilon^2\left(u_{xxxx} + \frac{1}{2}u_{xx}^3\right) \qquad \left(\text{where } \widetilde{\Gamma}(\alpha) = \Gamma\big(\tan^{-1}\alpha + \frac{\pi}{2}\big)\right). \tag{7}$$

In order to understand the convergence of the solution of (7) to that of (3), we are lead to the analysis of travelling and pulsating waves which are mathematically interesting in their own rights.

The description of these objects are most conveniently formulated in terms of the slope variable $v = u_x$, leading to the following equation:

$$v_t = \left(\widetilde{\Gamma}(v)v_x - \epsilon^2\left(v_{xxx} + \frac{1}{2}v_{xx}^3\right)\right)_x. \tag{8}$$

For *travelling wave*, we look for solutions of the form: $v(x,t) = V(x+ct)$. Then the function V solves

$$cV_x = \left[\widetilde{\Gamma}(V)V_x - \epsilon^2\left(V_{xxx} + \frac{1}{2}V_x^3\right)\right]_x \tag{9}$$

with $V \longrightarrow \theta_c^\pm$ "and" $V_x \longrightarrow m_\pm$ as $x \longrightarrow \pm\infty$. Integrating (9) leads to the *wave speed* c given by:

$$c = \frac{\left[\widetilde{\Gamma}(V)V_x - \epsilon^2\left(V_{xxx} + \frac{1}{2}V_x^3\right)\right]_{-\infty}^{\infty}}{\big[V\big]_{-\infty}^{\infty}} \longrightarrow_{\epsilon\to 0} \frac{\widetilde{\Gamma}(\theta_c^+)m_+ - \widetilde{\Gamma}(\theta_c^-)m_-}{\theta_c^+ - \theta_c^-}. \tag{10}$$

The existence of travelling waves and the above statement on the wave speed are proved rigorously using implicit function theorem, matching the stationary solution of (5) to the far-field conditions.

In order to analyze the situation when some initial slope lies within the range (θ_c^-, θ_c^+), we are lead to the study of the evolution of corrugated curves or "wrinkles". With the regularized dynamics (7), these lead to *pulsating waves — space time periodic solutions*. The interesting quantities to capture are the internal structure of the wrinkles and the *propagation speed of the boundary* between the wrinkled and non-wrinkled regions. These are analyzed asymptotically. The results are confirmed by numerical simulations.

The two figures illustrate some simulation results for the travelling and pulsating waves. (The functions plotted are the slope variables $v = u_x$.)

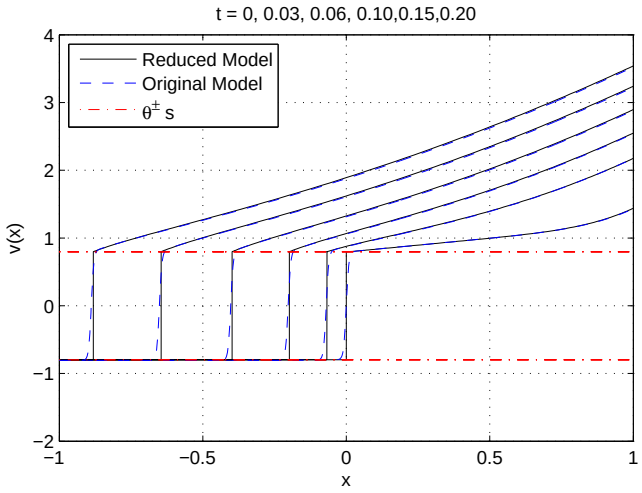

FIGURE 1. Time sequence comparison between the dynamics of the Reduced (3) and the Original (7) Models.

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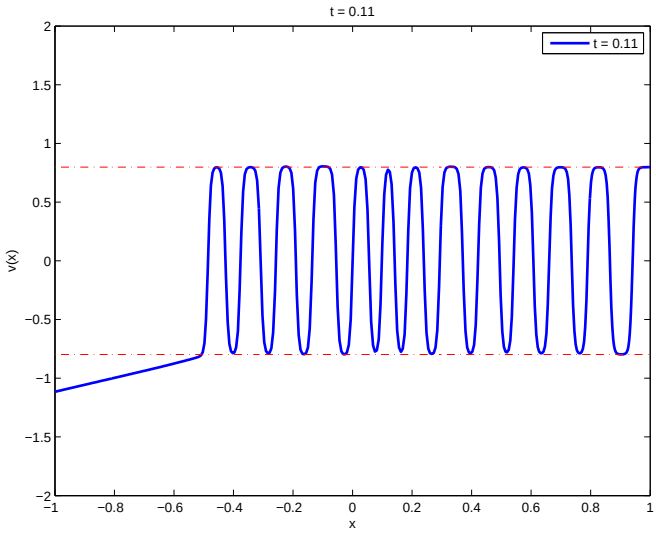

FIGURE 2. Internal structure of wrinkles and the boundary between wrinkled and non-wrinkled regions.

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Minimal configurations and sandpile measures

ANTAL A. JÁRAI
(joint work with Nicolás Werning)

Abelian sandpile model. Let $G = (V \cup \{s\}, E)$ be a finite, connected multigraph. For example, if $V \subset \mathbb{Z}^d$, we can form the *wired graph* G_V by identifying all vertices in $\mathbb{Z}^d \setminus V$ to a single vertex s. A *sandpile* on G is a collection of particles on the vertices in V, specified by a map $\eta : V \to \{0, 1, 2, \dots\}$. If $\eta(x) \geq \deg(x)$, we say that x is *allowed to topple*, meaning that x sends one particle along each edge incident with x. Thus when x topples, the configuration η is updated as follows:

$$\begin{aligned} \eta(x) &\longrightarrow \eta(x) - \deg(x); \\ \eta(y) &\longrightarrow \eta(y) + a_{xy}, \quad y \in V, y \neq x, \end{aligned} \tag{1}$$

where a_{xy} is the number of edges between x and y. Note that particles "arriving at s" are lost. We say that η is *stable*, if no vertex can topple, i.e. $\eta(x) < \deg(x)$ for all $x \in V$. Dhar [5] proved that any sandpile can be *stabilized* by carrying out

all possible topplings in some order until a stable configuration is reached, and the final stable configuration does not depend on the order of topplings chosen. The name "Abelian" is referring to this property.

We define a Markov chain on the collection of stable sandpiles as follows. At each time step, we add one particle at a uniformly random vertex in V, and stablize. There is a unique stationary distribution ν_G that is uniform on the collection $\mathcal{R}_G$ of recurrent states [5]. See the surveys [15] and [7] for further background.

Criticality. Sandpile models were introduced by Bak, Tang and Wiesenfeld as a toy example for *self-organized criticality* [2]. The Abelian sandpile is *critical*, in the sense known from lattice models of statistical physics (such as percolation and the Ising model): spatial correlations decay slowly, and various observables are conjectured to follow a power law distribution. For example, Majumdar and Dhar [12] proved that for all $d \geq 2$ we have

$$\lim_{V \uparrow \mathbb{Z}^d} \{\nu_V[\eta(x) = 0, \eta(y) = 0] - \nu_V[\eta(x) = 0]\nu_V[\eta(y) = 0]\} \sim c|x - y|^{-2d}, \tag{2}$$

as $|x - y| \to \infty$. A fascinating property of the model is that criticality appears here without having to set a parameter to a critical value [2], [5]. Some aspects of the 2D scaling limit are known rigorously; see [11], [6]

The burning bijection. Dhar's Burning Test [5] gives a simple algorithm that checks if a given stable sandpile is recurrent or not. Using this, Majumdar and Dhar [13] constructed a bijection between $\mathcal{R}_G$ and spanning trees of G. Note that under the bijection, ν_G is mapped onto the Uniform Spanning Tree measure, that we denote by μ_G. The burning bijection has been very useful in applying results about uniform spanning trees to the sandpile model; see [1], [10] and [8].

Minimal configurations. The proof of (2) is based on a determinantal formula that is valid more generally. Given $W \subset V$ and $\eta \in \mathcal{R}_V$, we denote by η_W the restriction of η to the subset W. We say that a configuration ξ in W is *minimal*, if there exists $\eta \in \mathcal{R}_V$ such that $\eta_W = \xi$, but $\eta - \delta_x \notin \mathcal{R}_V$ for any such η and any $x \in W$. (Here δ_x is the configuration with a single particle at x and no other particles.) Majumdar and Dhar [12] gave a method for writing the probability $\nu_V[\eta : \eta_W = \xi]$ as a determinant. If $V \subset \mathbb{Z}^d$, the entries of the determinant, in the limit $V \uparrow \mathbb{Z}^d$, are given in terms of the simple random walk potential kernel (if $d = 2$), or the simple random walk Green function (if $d \geq 3$).

Results. Based on the transfer-current theorem of Burton and Pemantle [4], an alternative determinantal formula can be given for minimal configurations. This has the advantage, that the limit of an infinite graph can be taken easily, since the limiting wired current exists by monotonicity [3].

Theorem 1. *Let $G = (V \cup \{s\}, E)$ be a finite multigraph, and let ξ be minimal on $W \subset V$. There exists a subset $\mathcal{E}$ of the set of edges touching W such that*

$$\nu_G[\eta : \eta_W = \xi] = \det(K_G(e, f))_{e,f \in \mathcal{E}}.$$

Here $K_G(e,f) = \delta(e,f) - Y_G(e,f)$, with Y_G denoting the transfer-current matrix and δ the identity matrix.

The above investigations led us to the following result on the thermodynamic limit of the Abelian sandpile model on very general graphs. Let $G = (V, E)$ be a locally finite, infinite graph, and $V_1 \subset V_2 \subset \cdots \subset V$ a sequence of finite sets such that $\cup_{n=1}^{\infty} V_n = V$. Let G_n denote the wired graph obtained from V_n. It is well-known that the uniform spanning tree measure μ_{G_n} converges weakly to a limit μ, called the Wired Uniform Spanning Forest measure on G, and this limit is independent of the sequence (V_n) [14], [3]. We say that an infinite tree *has one end*, if any two infinite paths in the tree have a finite symmetric difference.

Theorem 2. *Suppose that the each component of the Wired Uniform Spanning Forest on G has a single end almost surely. The measures ν_{G_n} weakly converge to a limit ν, that is independent of the sequence (V_n).*

We note that the assumption on one end cannot be omitted: Jarai and Lyons give a class of quasi one-dimensional graphs where there are exactly two extremal weak limits [9]. Earlier results on the thermodynamic limit of the Abelian sandpile model were based on giving a sort of extension of the bijection to the infinite graph, and assumed much more about the structure of the graph; see [1], [8].

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Strong approximation rates in the maximum-norm for noisy reaction–diffusion equations

Omar Lakkis
(joint work with Giorgos T. Kossioris and Marco Romito)

Introduction. Finite element methods for stochastic partial differential equations (meaning those of evolution type) have been the subject of a boom in the literature since the seminal paper of Allen, Novosel and Zhang (1998) [1, 2, 8, 9, 11, 7, 6].

We summarize here, to the best of our knowledge, a first derivation of maximum-norm (and other L_p norms) in space-time and strong in probability error estimates for the spatially discrete finite element approximation of reaction–diffusion (RD), semilinear parabolic, SPDE's with additive noise. Although we focus on the stochastic Allen–Cahn (SAC) equation, the techniques we present can be transported to a wider class of RD SPDE's. We have studied the SAC equation in [4] and this summary describes improved and novel error estimates of those therein. The full results will appear in a forthcoming paper [5].

Stochastic Allen–Cahn equation. Let $D = (-1, 1)$, $T > 0$, the solution of the *stochastic Allen–Cahn equation in one-dimension* is a (random) function $u : D \times [0, T] \to \mathbb{R}$ satisfy the following

$$\begin{gathered} \partial_t u(x,t) - \partial_{xx} u(x,t) + f_\epsilon(u(x,t)) = \epsilon^\gamma \partial_{xt} W(x,t) \\ \text{where } f_\epsilon(\xi) := \frac{1}{\epsilon^2}(\xi^3 - \xi) \text{ for } \xi \in \mathbb{R} \end{gathered} \tag{1}$$

with initial and boundary values

$$u(x,0) = u_0(x) \text{ and } \partial_x u(x,t)|_{x=\pm 1} = 0. \tag{2}$$

Here $\epsilon > 0$ is a "small" parameter, $\gamma \geq -1/2$, $\partial_{xt} W$ denotes *white noise* which we view, following [10], as a random measure on $D \times (0, T)$ such that

$$\int_A \partial_{xt} W(\mathrm{d}\, x, \mathrm{d}\, t) \in \mathrm{N}\,(0, |A|) \tag{3}$$

$$A \cap B = \emptyset \Rightarrow \int_A \partial_{xt} W \text{ and } \int_B \partial_{xt} W \text{ independent.} \tag{4}$$

An existing and unique solution u of (1) is studied in [3], in the mild sense, as a process that statisfies

$$\begin{aligned} u(x,t) &= \int_D G_t(x,y)u_0(y)\,\mathrm{d}\,y + \epsilon^\gamma z(x,t) \\ &\quad + \int_0^t \int_D G_{t-s}(x,y) f_\epsilon(u(y,s))\,\mathrm{d}\,y\,\mathrm{d}\,s \\ \text{where } z(x,t) &:= \int_0^t \int_D G_{t-s}(x,y)\partial_{ys} W(\mathrm{d}\,y, \mathrm{d}\,s), \end{aligned} \tag{5}$$

where G indicates the (Neumann boundary value) heat kernel and z satisfies

$$\partial_t z - \partial_{xx} z = \partial_{xt} W, \quad z(0,x) = 0, \text{ for } x \in D \quad \partial_x z(t, \pm 1) = 0. \tag{6}$$

Regularized approximation. To introduce a numerical solution, we first regularize (1) by replacing $\partial_{xt}W$ therein with an *approximate white noise* [4, for details] that is a random piecewise constant function on a cartesian decomposition in rectangles $D_m \times I_n$ of size $\sigma \times \rho$ of the space-time domain $D \times (0,T)$

$$\partial_{xt}\bar{W}(x,t) = \frac{1}{\sqrt{\sigma\rho}} \sum_{n=1}^{N} \sum_{m=1}^{M} \eta_{nm} \mathbf{1}_{D_m}(x) \mathbf{1}_{I_n}(t) \text{ where } \eta_{nm} \in \mathrm{N}\,(0,1)\,. \tag{7}$$

The *regularized solution* is defined as the function $\bar{u}$ solving the random PDE

$$\partial_t \bar{u}(x,t) - \partial_{xx}\bar{u}(x,t) + f_\epsilon(\bar{u}(x,t)) = \epsilon^\gamma \partial_{xt}\bar{W}(x,t) \text{ for } (x,t) \in D \times (0,T) \tag{8}$$

and the same initial and boundary values as for u in (2).

Galerkin finite-element solution. The semidiscrete (in space) finite element approximation is defined as the random function $U : (0,T) \to \mathbb{V}$, for an appropriate Galerkin finite element space $\mathbb{V}$ of meshsize h, as

$$\int_D \partial_t U(t)\Phi + \int_D \partial_x U(t)\partial_x \Phi + \int_D f_\epsilon(U(t))\Phi = \int_D \partial_{xt} W(t)\Phi. \tag{9}$$

This is an SDE with values in $\mathbb{V}$.

Error estimates: a roadmap. As noted in [1], a natural way to obtain an error estimate, with rates, for the error $u - U$, in a norm $\|\cdot\|$, say, is to decompose the job into two steps:

(1) Bound $\|u - \bar{u}\|$: the error between the exact solution of (1) and the approximate solution of (8), with respect to the regularization parameters σ and ρ. This step requires a combination of PDE techniques with probabilistic arguments.
(2) Bound $\|\bar{u} - U\|$: the error between the regularized solution and its numerical approximation. This step draws from "classical" numerical analysis and the main ingredients to obtain error rates are the *approximation power* of $\mathbb{V}$ as well as the regularity of $\bar{u}$. This regularity must be quantified, via upper bounds, that are the finest possible with respect to σ and ρ.

In [1] and other cited works, the norm that is used is $\mathbb{E}\|u-U\|_{\mathrm{L}_2(D\times(0,T))}$. Here we work with a more general norm $\mathbb{E}\|u-U\|_{\mathrm{L}_p(D\times(0,T))}$, with $p\in[2,\infty]$. The motivation for this is that in the Allen–Cahn problem it is curcial to track the interface and the L_2 norm is too weak to quantify anything useful about an interface. The Sobolev H^1 (semi) norm is too strong, and no convergence is expected in that norm, so L_∞ appears to be the best compromise.

Exact-to-regularized strong convergence theorem. *Let u and $\bar{u}$ be stochastic processes solutions on a time interval $[0,T]$ to (1) and (8), respectively. Then for every $p\geq 2$ and every $\kappa>0$, there is C_1 depending only on p,T,ϵ,κ such that*

$$\mathbb{E}\big[\|u-\bar{u}\|^p_{L^\infty((0,T)\times D)}\big]\leq \frac{C_1T}{\epsilon^2}\,\mathrm{e}^{\frac{6p}{\epsilon^6}T}(\rho^{1/2}+\sigma)^{\frac{p}{2}(1-\kappa)}, \tag{10}$$

The proof of this result rests on the decomposition of the type

$$u=v+\epsilon^\gamma z,\bar{u}=\bar{v}+\epsilon^\gamma\bar{z}\text{ with }z\text{ defined by (6)}, \tag{11}$$

$\bar{z}$ being a similar process but with $\partial_{xt}W$ replaced by $\partial_{xt}\bar{W}$ and careful bounds of both z and the *stochastically shifted solution* v.

Regularity estimates theorem. *For every $p\in[2,\infty)$ and $\kappa>0$ there is a constant $C_2>0$, depending on p,ϵ only, and C_3 depending on p,ϵ,κ only such that*

$$\begin{gathered}\mathbb{E}[\|\partial_t\bar{u}\|^p_{\mathrm{L}_p((0,T)\times D)}]\vee\mathbb{E}[\|\partial_{xx}\bar{u}\|^p_{\mathrm{L}_p((0,T)\times D)}]\leq C_3\Big[\rho^{-\frac{3}{4}p}+\rho^{-\frac{p}{2}}\sigma^{-\frac{p}{2}}\Big],\\ \mathbb{E}\sup_{[0,T]}\|\partial_{xx}\bar{u}\|_{\mathrm{L}_p(D)}\leq C_4\Big[\rho^{-\frac{3}{4}-\kappa}+\rho^{-\frac{1}{2}-\kappa}\sigma^{-\frac{1}{2}}\Big]\end{gathered} \tag{12}$$

It is worth noting that the right hand side in these regularity estimates explodes as $\rho,\sigma\to 0$. This is to be expected as otherwise, $\bar{u}\to u$ in spaces where u does not exist. What is important about this result, is the *rates* in ρ and σ at which the norms explode.

Regularized-to-numerical error estimates theorem. *For each $\mu>0$ there exists a C_5 which depends on μ and is a linear combination of the (semi)norms of $\bar{u}$ appearing in (12) times an exponential in ϵ of the type appearing in (10)*

$$\|\bar{u}(t)-U(t)\|_{\mathrm{L}_\infty(D)}\leq C_5h^{2-\mu}\log h\log t. \tag{13}$$

Conclusion. By combining the above results and coupling appropriately h,ρ and σ, the spatially discrete Galerkin finite element solution U, provided infintely precise Monte-Carlo approximation in the probability space, is seen to converge with a rate of $h^{1/2-\kappa}$ and a constant depending on κ and growing exponentially with $1/\epsilon^2$.

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Time-evolution of Probability Measures on Collision Trees – a Tool for Micro-macro Transitions

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(joint work with Florian Theil)

Deriving continuum models as a scaling limit of atomistic particle dynamics is a fundamental problem of mathematical physics. The aim is to prove the validity of continuum equations like the Boltzmann equation to describe the effective behavior of deterministic many particle dynamics. The first rigorous derivation of the Boltzmann equation was given by Lanford [2] for short times using the BBGKY hierarchy, also see [1] and references therein.

Instead of classical hard-sphere dynamics, we use the simplification of ballistic annihilation, where particles are removed after their first collision. The initial states are random, i.e. the initial configuration of n particles in the phase space $U \times \mathbb{R}^d$ (with $U = \mathbb{T}^d$ the unit torus) are drawn independently according to some density $f_0 \in L^1(U \times \mathbb{R}^d)$. Then the dynamics are deterministic. As long as they are intact ($\beta = 1$) the centres of the spheres move along straight lines with constant

velocity. When the centres of two spheres, which are still intact, come within distance a, then both spheres are destroyed ($\beta = 0$). We are interested in the behaviour for $n \to \infty$ for the Boltzmann-Grad scaling

$$na^{d-1} = 1.$$

In this limit the density f solves the nonlinear Boltzmann equation

$$\partial_t f + v \cdot \nabla_u f = -Q_-[f, f], \tag{1}$$

such that for all open sets $A \subset U \times \mathbb{R}^d$ and any given time, the number of particles in A divided by the total number of particles converges to $\int_A f(u, v, t)\, \mathrm{d}u\, \mathrm{d}v$. Here $Q_- \geq 0$ is the collision operator accounting for the losses. Particles with velocities v and v' collide at position u with a given probability depending on v and v' and impact parameter $\nu \in S^{d-1}$. In the density there is a loss at (u, v) and (u, v'). The loss-operator has the form

$$Q_-[f, f](u, v) = \int_{\mathbb{R}^d} \int_{S^{d-1}} f(u, v')\, f(u, v)\, [(v - v') \cdot \nu]_+ \, \mathrm{d}\nu\, \mathrm{d}v'.$$

In the full hard-sphere dynamics, there is another term Q_+ accounting for particles with changed velocity after a collision, which can be seen as an immediate creation of new particles at different points in phase space after the removal of particles in a collision.

In [4], we develop a novel approach for the scaling limit using probability measures on collision trees way both for empiric probabilities due to the many particle flow as well as for the idealized behaviour suggested by the Boltzmann equation. In [3] we analyzed the situation of spatially homogeneous initial data with f_0 independent of u, such that the corresponding version of (1) does not include the transport term $v \cdot \nabla_u f$. In the homogeneous case it was possible to give explicit expressions for the time-dependent probabilities.

We consider collision trees as marked trees $\mathcal{MT}$ where each node of a tree Φ has collision time s, initial velocity v and collision parameter ν as a label.

The idealized probability measures P_t are introduced via the Kolmogorov equation

$$\begin{cases} \frac{\partial P_t}{\partial t} & = \mathcal{Q}_t[P_t, P_t, \mu_t[P_t]], \\ P_0 & = f_0 \end{cases} \tag{2}$$

where the collision rate $\mu_t[P] \in M(\mathcal{MT})$ (the space of unsigned Radon measures) is defined by

$$\mu_t[P](\Phi) = \int_{S^{d-1}} \mathrm{d}\nu \int_{\mathcal{MT}} \mathrm{d}P(\Psi)\, \delta(u - u(\Psi) + t(v - v(\Psi)))\, [(v - v(\Psi)) \cdot \nu]_+,$$

and $\mathcal{Q}_t[P, P', \mu]$ is given by

$$\begin{aligned} \mathcal{Q}_t[P,\, P',\, \mu](\Phi) &= P(\bar{\Phi}_t)\, L_t[P'_t](\Phi), \\ L_t[P',\, \mu](\Phi) &= \delta(t - \tau(\Phi))\, P'(\Phi'_t)\, [(v - v') \cdot \nu_t]_+ - \mu(\Phi), \end{aligned}$$

with the convention at a collision at a time t, the previous tree is denoted by $\bar{\Phi}_t$ and the colliding tree with Φ'_t with $v = v(\Phi)$, $v' = v(\Phi'_t)$ etc. Note that the operator L_t

extracts subtrees which collide with the root particle. Using semigroup methods, it is possible to show that (2) is well-posed for suitable f_0.

A similar Kolmogorov equation can be also derived for the empirical probability measures $\hat{P}_t^a$ as long as certain rare events like recollisions and resonance effects can be excluded. A comparison of these two equations then leads to $\lim_{a\to 0} \|P_t^a - \hat{P}_t\|_{L^1(\mathcal{MT})} = 0$. This is enough to deduce the main result:

The density of the unscattered particles converges to a solution of the Boltzmann equation in the sense that for all $\varepsilon > 0$ and all open $A \subset U \times \mathbb{R}^d$ uniformly for t in a compact set

$$\lim_{a\to 0} \mathrm{Prob}_a \left(\left| \frac{1}{n} \# \left\{ i \;\middle|\; (u_i(t), v_i(t)) \in A,\, \beta_i^{(a)}(t) = 1 \right\} - \int_A \mathrm{d} f_t(u,v) \right| > \varepsilon \right) = 0,$$

where $f_t(\,\cdot\,,\,\cdot\,) = f(\,\cdot\,,\,\cdot\,,t)$ is the unique mild solution of (1). Furthermore, there exists a sequence $a_k \to 0$ and corresponding particle numbers n_k, such that with probability 1,

$$\frac{1}{n_k} \sum_{i=1}^{n} \beta_i^{(a_k)}(t)\, \delta(\,\cdot\, - (u_i(t), v_i(t))) \overset{*}{\rightharpoonup} f_t$$

weak-$*$ in $M(U \times \mathbb{R}^d)$ as $k \to \infty$, with δ denoting the Dirac distribution.

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