DFG FORSCHERGRUPPE 718

Closing Workshop

March 20 – 22 2013 Leipzig

Schedule

		WED 20th	THURS 21st	FRI 22nd
Venue: Max Planck Institut, Inselstraße 22, Room G10				
	10.00		**Giacomin**	**Peletier**
	11.00		**Biskup**	**Cerny**
	12.00		**Niethammer**	**Carlen**
		(13.45 Opening)		(13.00 Closing)
	14.00	**Norris**		
	15.00	**Lewin**	**Mielke**	
	16.00	Coffee Break	Coffee Break	
	16.30	**Orlandi**	**Lelievre**	
	17.30	**Ueltschi**	**Caravenna**	
	19.30	**Conference Dinner***		

* Panorama Restaurant, Augustusplatz, Registration Required

BERLIN-LEIPZIG WORKSHOP MARCH 2013
TALKS AND ABSTRACTS

Marek Biskup: Law of the extremes for the two dimensional discrete Gaussian Free Field

Abstract: A two-dimensional discrete Gaussian Free Field (DGFF) is a Gaussian process indexed by the vertices in a finite set, e.g., a square, in the square lattice. The process is centered (mean zero) and the covariance is given by the Green function of the simple random walk killed upon exiting from the set. Recently, much effort has been paid to the study of the concentration properties and tail estimates for the maximum of DGFF. I will address the limit law of the whole extreme-order statistics of the DGFF as the square-size tends to infinity. In particular, I will show that the extremes converge in law to a randomly-shifted Gumbel Poisson point process which is decorated, independently around each point, by a random collection of auxiliary points. The random shift arises from a random measure that characterizes the joint law of the value and position of the extremes of the DGFF. This random measure encodes many intriguing properties of the DGFF, e.g., Gibbs-Markov property and conformal invariance. This talk is based on joint work with Oren Louidor (UCLA).

Francesco Caravenna: Scaling Limits and Universality for Random Pinning Models.

Abstract: We consider the so-called random pinning model, which may be described as a Markov chain that receives a random reward/penalty each time it visits a given site. When the return time distribution of the Markov chain has a polynomial tail, with exponent larger than $1/2$, the model is said to be disorder-relevant, since an arbitrarily small amount of external randomness (quenched disorder) changes radically the critical properties of the model. In this regime, we show that the partition function of the model, under an appropriate weak coupling scaling limit, converges to a universal quantity, given by an explicit Wiener chaos expansion. This quantity can be viewed as the partition function of a universal "continuum random pinning model", whose construction is part of our approach.
Joint work with Nikos Zygouras and Rongfeng Sun

Eric Carlen: Optimal mass transportation in non-commutative probability

Abstract: We introduce a metric on the space of density matrices for an N- fermion system that is the analog of the 2-Wasserstein metric. In particular, we show that the fermionic Fokker-Planck evolution is gradient flow for the von Neumann entropy in this metric, and prove a Talagrand inequality. Several open problems are discussed.
This is joint work with Jan Maas.

Jiri Cerny: t.b.a.

Giambattista Giacomin: Synchronization and random long time dynamics for interacting rotators

Abstract: The talk will focus on the dynamics of classical mean field plane rotator model, in the phase transition regime. In the limit of infinitely many rotators and for finite times, the empirical measure of the system is accurately described by a non-linear and non-local Fokker-Planck PDE. However if we focus on a large but finite number N of rotators, it is natural to wonder whether the PDE approximation is still reliable and up to which times. I will present results on the finite N dynamics that establish on which time scale the PDE approximation breaks down. The dynamics on the new time scale is random, but it can be accurately described in terms of a diffusion on the manifold of stationary solutions of the Fokker-Planck PDE.

Tony Lelievre: Numerical methods in molecular dynamics.

Abstract: Molecular dynamics is now a very widely used tool to study the matter at the molecular level. It is used in various fields, such as biology, chemistry or materials science. The aim is in particular to understand the relationships between the macroscopic properties of a molecular system and its atomistic features. For example, one would like to compute the constitutive relations for materials from molecular models, or predict the most likely conformations of a protein in a solvent from its amino acid sequence. One of the difficulty to reach this aim is related to timescales: the typical timescale of a molecular dynamics simulation is much smaller than the typical timescale at which the crucial events, from a macroscopic viewpoint, occur. This is related to the metastability of a molecular dynamics trajectory: the system stays for a very long time in some regions of the configuration space (called metastable state), before hopping to another one, and it is difficult to observe and simulate such rare events. An associated feature is the multimodality of the statistical ensemble (a probability measure) sampled by the molecular dynamics trajectories. Many methods have been proposed in the molecular dynamics community to deal with these difficulties, and we will focus on two prototypical ones for which a mathematical analysis gives useful insights. We will first present adaptive importance sampling techniques, which have been proposed to sample efficiently statistical ensembles. Then, we will propose a mathematical analysis of the parallel replica algorithm which has been introduced by A.F. Voter to generate efficiently metastable dynamics.

Mathieu Lewin: Large quantum systems in the mean-field regime: Hartree and Bogoliubov theories

Abstract: We consider the limit of a large number N of bosons described by the many-body Schrödinger equation. We work in the mean-field regime, which means that the interaction is of order $1/N$. Under some general assumptions, we prove that the eigenvalues of the Schrödinger Hamiltonian are given to first order by the nonlinear Hartree theory, and to second order by Bogoliubov's theory.
This is a review of recent works with Phan Thanh Nam (Cergy), Nicolas Rougerie (Grenoble), Sylvia Serfaty (Paris) and Jan Philip Solovej (Copenhagen).

Alexander Mielke: On entropy-driven dissipative quantum mechanical systems

Abstract: Pure quantum mechanics can be formulated as a Hamiltonian system in terms of the density matrix. The von Neumann entropy can be used to model dissipative effects, in particular for the coupling to dissipative macroscopic systems such as heat baths. Following Öttinger (2010) we use the GENERIC framework (General Equations for Non-Equilibrium Reversible Irreversible Coupling) to construct thermodynamically consistent evolution equations as a sum of a Hamiltonian and a gradient-flow contribution.
The dissipation mechanism is modeled via the canonical correlation operator, which is the inverse of the Kubo-Mori metric for density matrices and which is strongly linked to the von Neumann entropy for quantum systems. Thus, one recovers the dissipative double-bracket operators of the Lindblad equations but encounters a correction term for the consistent coupling to the dissipative dynamics.
One of our models couples a quantum system to a finite number of heat baths each of which is described by a time-dependent temperature. We discuss general existence results and provide sufficient conditions that guarantee the convergence of all solutions into thermal equilibrium.

References: A. Mielke. Dissipative quantum mechanics using GENERIC, WIAS preprint 1710, 2012. To appear in "Proceedings of the conference "Recent Trends in Dynamical Systems", 2013.

Barbara Niethammer: Kramers- and non-Kramers phase transitions in a nonlocal Fokker-Planck equation

We discuss a nonlocal Fokker-Planck equation that describes energy minimisation in a double well-potential and is driven by a time-dependent constraint. Via formal asymptotic analysis we identify different small parameter regimes and derive reduced dynamical models that describe hysteretic and non-hysteretic phase transitions.
This is joint work with Michael Herrmann and Juan Velazquez.

James Norris: A consistency estimate for Kac's model of elastic collisions in a dilute gas

Abstract: With high probability, the empirical distribution of velocities does not depend on the number of particles N, up to a tolerance of order $N^{-1/10}$ in Wasserstein distance.

Enza Orlandi: Local and nonlocal Ginzburg-Landau functionals with random external field minimizers and interfaces

Abstract: I will present some results regarding minimizers and interfaces of local and nonlocal Ginzburg-Landau functionals perturbed by an additive external random field. In particular I will consider a small random perturbation of the energy functional

$$\|u\|^2_{H^s(\Lambda,\mathbb{R}^d)} + \int_\Lambda W(u)dx$$

for $s \in (0,1)$, where the non-local part $\|u\|^2_{H^s(\Lambda,\mathbb{R}^d)}$ denotes the contribution coming from

$\Lambda \Subset \mathbb{R}^d$ to the $H^s(\mathbb{R}^d)$ (semi)norm of u, and W is a double well potential. There exists, as Λ invades $\mathbb{R}^d$, for almost all realizations of the random term a minimizer, which is unique under compact perturbations, when $d = 2$, $s \in (\frac{1}{2}, 1)$ and when $d = 1$, $s \in [\frac{1}{4}, 1)$. This uniqueness is a consequence of the randomness. When the random term is absent, there are two minimizers which are invariant under translations in space, $u = \pm 1$.
In collaboration with Nicolas Dirr (Cardiff University).

Mark Peletier: Exact crystallization in a block copolymer model

Abstract: One of the holy grails of material science is a complete characterization of ground states of material energies. Some materials have periodic ground states, others have quasi-periodic states, and yet others form amorphic, random structures. Knowing this structure is essential to determine the macroscopic material properties of the material. In theory the energy contains all the information needed to determine the structure of ground states, but in practice it is extremely hard to extract this information.
In this talk I will describe a model for which we recently managed to characterize the ground state in a very complete way. The energy describes the behaviour of diblock copolymers, polymers that consist of two parts that repel each other. At low temperature such polymers organize themselves in complex microstructures at microscopic scales.
We concentrate on a regime in which the two parts are of strongly different sizes. In this regime we can completely characterize ground states, and even show stability of the ground state to small energy perturbations.
This is work with David Bourne and Florian Theil.

Daniel Ueltschi: Random loop representations for quantum spin systems

Abstract: Certain quantum spin systems have fascinating random loop representations that allow to express the quantum correlations in a probabilistic way. I will describe an extension of the representations of Toth and Aizenman-Nachtergaele for the ferromagnetic and antiferromagnetic Heisenberg models. The representation allows to prove the existence of a phase transition with magnetic long-range order in a quantum spin 1 system. It also allows to formulate conjectures about the nature of the phase transition, which is still not understood.