CPP 19: SYMPOSIUM Driven Soft Matter IV

Time: Wednesday 14:00–16:00 Location: C 130

CPP 19.1 Wed 14:00 C 130

Simulating rare events in nonequilibrium systems: nucleation in a driven Ising system — •Rosalind Allen — SUPA School of Physics, Edinburgh University, Edinburgh, UK

I will describe the application of the recently developed Forward Flux Sampling method [1-4] for simulating rare events to a nonequilibrium transition - nucleation in a sheared two dimensional Ising system. I will describe an analysis of the transition state ensemble to understand the reaction mechanism and rationalise the observed nonmonotonic dependence of the nucleation rate on the shear rate.

[1] Sampling rare switching events in biochemical networks. R. J. Allen, P. B. Warren and P. R. ten Wolde, Phys. Rev. Lett. 94, 018104 (2005)

[2] Simulating rare events in equilibrium or nonequilibrium stochastic systems. R. J. Allen, D. Frenkel and P. R. ten Wolde, J. Chem. Phys. 124, 024102 (2006)

[3] Forward flux sampling-type schemes for simulating rare events: Efficiency analysis. R. J. Allen, D. Frenkel and P. R. ten Wolde, J. Chem. Phys. 124, 194111 (2006)

[4] Computing stationary distributions in equilibrium and nonequilibrium systems with forward flux sampling. C. Valeriani, R. J. Allen, M. Morelli, D. Frenkel and P. R. ten Wolde, J. Chem. Phys. 127, 114109 (2007)

CPP 19.2 Wed 14:15 C 130

Driven polymer blends: criticality and structure formation in inhomogeneous temperature fields — •Werner Köhler, Albert Voit, and Alexei Krekhov — Physikalisches Institut, Universität Bayreuth

Even moderately inhomogeneous temperature fields, as generated by localized laser heating, couple to the order parameter (the composition) and can drive polymer blends far out of equilibrium. Close to the critical point this Soret effect can be four to five orders of magnitude stronger than in conventional liquid mixtures. Global equilibrium phase diagrams loose their meaning, and even UCST-mixtures can be quenched into phase separation by local heating. Close to the critical point we observe critical scaling, and almost arbitrary composition patterns can be written into a PDMS/PEMS blend using a galvano laser scanner. Below the spinodal the prescribed patterns compete with the intrinsic length scale of the correlation length, and surface tension effects become increasingly important. The theoretical modelling of the structure formation is based on a modified Cahn-Hilliard-equation, and 2D-models are able to reproduce the essential spatio-temporal features. While the susceptibility (Soret coefficient) diverges at the critical point of the liquid-liquid phase transition, it is completely insensitive to a glass transition due to a cancellation of local friction being effective on the molecular length scale of a few monomers.

[1] A. Voit, A. Krekhov, W. Enge, L. Kramer, W. Köhler, PRL 94 (2005) 214501; [2] A. Voit, A. Krekhov, W. Köhler, Macromolecules 40 (2007) 9; [3] A. Voit, A. Krekhov, W. Köhler, PRE 70 (2007) 011808

CPP 19.3 Wed 14:30 C 130

Super-heterodyne light scattering as versatile tool to characterize multiphase flow — •Thomas Palberg[1], Tetjana Köller[1], and Gerhard Nägele[2] — [1]Institut f. Physik, Johannes Gutenberg Universität, Mainz — [2]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH., Jülich

Condensed matter put to extreme mechanical impact may react by crack formation, creep flow or even (partial) melting behaviour. Soft matter model systems may help in elucidating such phenomena due to both their softness, implying significant mechanical response even for small loads and their enlarged length and time scales, facilitating convenient optical access. Colloidal crystals in particular may display shear induced straining, local or global shear melting or shear induced crystallization, if subjected to shearing fields. Structural evolution may be monitored in detail using either video microscopy or time resolved static light scattering. We here show that incoherent scattering contributions (dominant at low scattering angles or selectively detected in VH geometry) can be exploited to provide the complementary information on the complex flow behaviour, without interference with the structural distribution. Super heterodyning in addition renders the data of interest free of homodyne contributions and low frequency noise. The combination of coherent and incoherent scattering experiments therefore may help in clarifying the coupling between structure and motion under shear. We exemplify our method studying an aqueous charged sphere suspension driven under the influence of different fields.

CPP 19.4 Wed 14:45 C 130

Fluid interfaces under shear: Studying the Ising model under drive. — Tom Smith[1], Oleg Vasilyev[2], Douglas B. Abraham[3], •Anna Maciolek[2], and Matthias Schmidt[1] — [1]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK — [2]Max-Planck-Institut fuer Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany — [3]Theoretical Physics, Department of Physics, University of Oxford

We use a phase-separated driven two-dimensional Ising lattice gas in order to model liquid-liquid interfaces exposed to shear flow parallel to the interface. The model is confined between two parallel walls and two different types of external field with direction parallel to the walls are used to drive the system out-of-equilibrium : i) the field acts locally at the walls, or ii) the field varies linearly with distance across the slit. From computer simulations using Kawasaki (conserved order parameter) dynamics we obtain structural information such as the lateral and transversal correlation lengths at the interface. In equilibrium the confinement of the interface due to the presence of walls reduces its width and the characteristic transverse (correlation) length, while increasing the interfacial free energy. We find that shear induces similar effects. Furthermore we test whether the roughness of the driven interface decreases as compared to the equilibrium case. The global effects of shear on the system are in particular surprising for case i) where only particles at the boundaries of the system are driven. The relationship of our findings to recent experimental results in sheared phase-separated colloidal dispersions is discussed.

CPP 19.5 Wed 15:00 C 130

2d-Motion of magnetic particles in external fields — •Artur Erbe, Peter Henseler, Michael Koeppl, Marcin Zientara, Peter Nielaba, and Paul Leiderer — Universitaet Konstanz, FB Physik, Konstanz, Germany

Magnetic colloidal particles are ideal model systems to study the behavior of particles, which interact via dipole-dipole interactions, under various conditions. Here we present studies of a two-dimensional system of micron-sized particles moving under the influence of an external field. The external force acting on the particles is either given by gravity or a gradient in the magnetic field. We study the motion of the particles by video microscopy and compare the results to molecular dynamics simulations. Layering and layer-reduction effects are observed, when the particles are driven through narrow channels. This behavior is explained by the interplay of the interparticle interactions and the influence of the confining walls. In unbounded systems we observe laning of the particles. We discuss possible origins for this behavior.

CPP 19.6 Wed 15:15 C 130

Bridging scales in a phase separating binary fluid: From Cahn-Hilliard to Doi-Ohta model — •Asja Jelić, Patrick Ilg, and Hans Christian Öttinger — ETH Zurich, Department of Materials, Polymer Physics, CH-8093, Switzerland

Mixtures of immiscible fluids are systems that can be studied at various length and time scales. The General Equation for the Non-Equilibrium Reversible-Irreversible Coupling (GENERIC) framework is used to connect two different levels of description of a phase separating binary fluid. We start from the Cahn-Hilliard model of spinodal decomposition in a binary fluid mixture under flow from which we derive the coarse-grained description. The familiar Doi-Ohta model is recovered in the long wavelength limit. The key ingredient required for this procedure is a mapping of the variables of one level to another, so that a statistical formulation of GENERIC framework in a generalized mixed ensemble enables one to develop a thermodynamically consistent formulation and simulation algorithms for non-equilibrium systems and sets the framework for their multi-level description. The present state of the study relates the two levels by giving the expected reversible time evolution and shedding new light on the irreversible processes and the interpretation of the parameters in the Doi-Ohta model.

CPP 19.7 Wed 15:30 C 130

Thermodynamically consistent coarse-graining in unentangled polymer melts: mapping microscopic dynamics to conformation tensor theory — •Patrick Ilg, Martin Kröger, and Hans Christian Öttinger — ETH Zürich, Polymer Physics, 8093 Zürich, Switzerland

The dynamics of polymer melts both, in equilibrium and under flow is extremely interesting from a theoretical and application point of view. We here propose a systematic and thermodynamically consistent coarse-graining method that uses a combination of Monte-Carlo and molecular dynamics simulations in order to break the time-scale problem present in polymer systems. The method relies on the splitting of reversible and irreversible contributions to the dynamics and explicitly accounts for the entropy generated in the coarse-graining step. This work uses a general framework of nonequilibrium thermodynamics [1] and builds upon similar studies on the derivation of hydrodynamics for rarefied gases [2].

Starting with a classical bead-spring model of unentangled polymer melts, we coarse-grain to the frequently used conformation tensor level. We verified the method for the case of planar shear flow, where we obtain the correct viscosity and normal stress differences in the low shear rate regime.

[1] H. C. Öttinger. Beyond-Equilibrium Thermodynamics. Wiley, 2005. [2] M. Kröger and H. C. Öttinger. Beyond-equilibrium molecular dynamics of a rarefied gas subjected to shear flow. J. Non-Newtonian Fluid Mech., 120:175–187, 2004.

CPP 19.8 Wed 15:45 C 130

Correlations in granular media with volume driving — •Wolf Till Kranz[1], Timo Aspelmeier[1], and Annette Zippelius[1,2] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen — [2]Universität Göttingen

Due to the dissipative nature of the interaction of granular particles an input of energy is needed in order to reach a stationary state. The simplest example of energy injection, volume driving by randomly forcing each particle, leads to an unphysical divergence of the structure factors at long wavelengths. We show that this divergence is removed when the driving is modified to obey momentum conservation. The length scale l on which momentum is conserved determines the length scale on which correlations build up: on lengths scales shorter than l the remnants of the divergence are still visible while it is suppressed on longer scales. We discuss the long wavelength behaviour of the static structure factor and the longitudinal current correlation function.