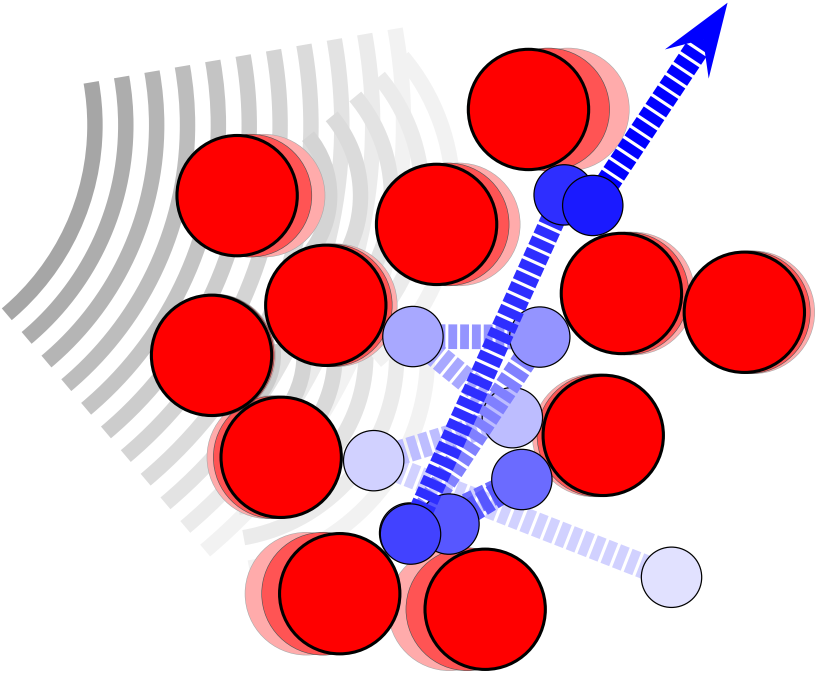
Complex transport in strongly interacting systems



Munich, July 25-27 2012

Arnold Sommerfeld Center for Theoretical Physics

organizers
Erwin Frey (LMU München)
Thomas Franosch (Erlangen)

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In recent years our understanding of the slowing down of transport in by repeated scattering from neighboring particles or obstacles has increased rapidly and mechanims have been identified leading to striking phenomena such as the glass transition, jamming, and the localization transition. The purpose of the workshop is bring together the different communities working on these related questions and to promote and transfer concepts to establish a broader picture of complex slow processes.

The focus of the meeting will be put on recent developments of the glass transition to more complex systems, such as gelation, polymers, colloids under shear, and granular systems, as well as jamming and dense active matter, and their comparision to the localization transition of classical particles and waves. The scope includes both theory and computer simulations which will complemented by experiments.

General Information

Directions

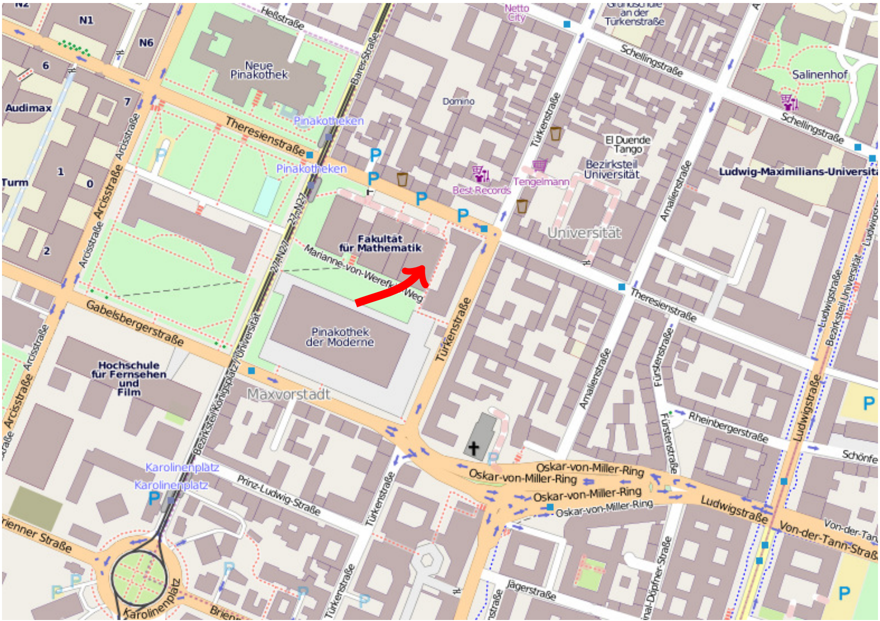
The conference takes place in the
Sommerfeld lecture hall A348/349 (3rd floor)
Arnold Sommerfeld Center for Theoretical Physics
Theresienstr. 37
D-80333 München

From the train station (Hauptbahnhof):

- Take the bus 100 leaving from the north site of the station.
- Get out at bus stop "Pinakotheken"
- Cross "Gabelsberger Straße" and walk 200m along "Barer Straße"
- Enter the building on the right site.

From the airport (Flughafen):

- Train S1 or S8 direction City Center (Innenstadt) till station Karlsplatz(Stachus)
- Then change and take the tram 27 (Petuelring)
- exit station "Pinakotheken" (3 stations)



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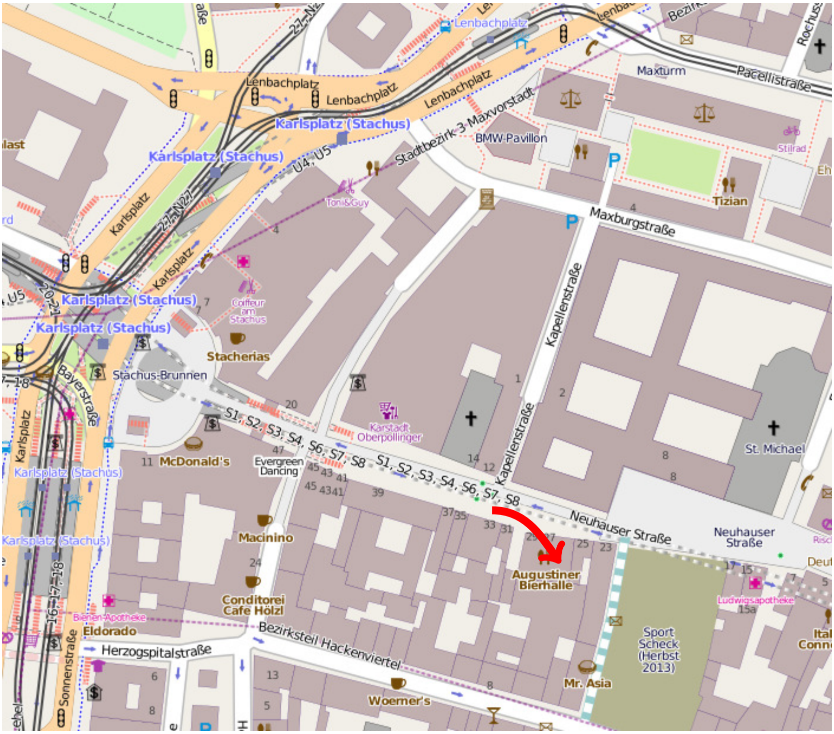
Conference Dinner

The conference dinner is on Thursday, 26 July, 19:30 at
‘Zum Augustiner’
Neuhauserstr. 27
80331 München

5 min to walk from the Karlsplatz (Stachus) train station / bus stop.

There will be Bavarian buffet and draught beer.



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	Wednesday July 25	**Thursday** July 26	**Friday** July 27
08:45	welcome		
09:00	com. transp. ordered syst. T. Lubensky R. Schilling K. Binder chair: E. Frey	complex rheology J. Horbach S. Egelhaaf M. Fuchs chair: Schirmacher	anomalous transport R. Metzler F. Höfling G. Maret chair: Voigtmann
10:30	coffee break	coffee break	coffee break
11:00	slow transp. heterog. str. V. Krakoviack E. Del Gado G. Szamel chair: W. Kob	fast dynamics P. Lunkenheimer E. Rößler W. Schirmacher chair: R. Pick	granular matter 2 H. Herrmann J.-L. Barrat M. Sperl chair: Franosch
12:30	lunch break	lunch break	closing remarks
14:00	granular matter 1 A. Zippelius C. Heussinger chair: Wagner	glass transition W. Kob A. Moreno F. Zamponi chair: Krakoviack	
15:00	gels and networks E. Bartsch F. Sciortino chair: Wagner		
15:30		coffee break	
16:00	coffee break	diffusion A. Meyer J. Baschnagel L. Cipelletti chair: W. Petry	
16:30	active systems A. Bausch H. Löwen chair: M. Fuchs		
17:30			
19:30		**conference dinner**	
	Wednesday July 25	**Thursday** July 26	**Friday** July 27

Wednesday

08:45 – 09:00 Opening and Welcome

Erwin Frey, Thomas Franosch

09:00 – 10:30 Complex Transport in Ordered Systems

Chair: Erwin Frey

A1	**Tom Lubensky**	*Zero modes, states of self stress, and surface phonons in periodic networks*
A2	**Rolf Schilling**	*Spreading of localized excitations*
A3	**Kurt Binder**	*Modeling transport in confined colloidal crystals in equilibrium and under compression and shear deformations*

10:30 – 11:00 Coffee break

11:00 – 12:30 Slow Transport in Heterogenous Structures

Chair: Walter Kob

B1	**Vincent Krakoviack**	*Mode-coupling theory, quenched randomness and self-generated disorder*
B2	**Emanuela Del Gado**	*Heterogeneous glasses and sustainable cement*
B3	**Grzegorz Szamel**	*Glassy dynamics of partially pinned fluids:* *an alternative mode-coupling approach*

12:30 – 14:00 Lunch break

14:00 – 15:00 Granular Matter I

Chair: Herbert Wagner

C1	**Annette Zippelius**	*Cohesive Granular Fluids*
C2	**Claus Heussinger**	*Jamming and glassy dynamics in driven granular systems:* *"melting a glass by freezing"*

15:00 – 16:00 Gels and Networks

Chair: Herbert Wagner

D1	**Eckhard Bartsch**	*Influence of particle softness and attraction range on gel and glass transitions in colloidal microgel susp. with short-ranged depletion attraction*
D2	**Francesco Sciortino**	*Re-entrant phase behavior of network fluids:* *A patchy particle model with temperature-dependent valence*

16:00 – 16:30 Coffee break

16:30 – 17:30 Active Systems

Chair: Matthias Fuchs

E1	**Andreas Bausch**	*Cytoskelotal pattern formation: Self organization of driven filaments*
E2	**Hartmut Löwen**	*Transport in strongly interacting active colloids*

A1 **Tom Lubensky** **09^{00} – 09^{30}**

Zero Modes, States of Self Stress, and Surface Phonons in Periodic Networks

Tom Lubensky,[1,*] Kai Sun,[2] Xiaoming Mao,[1] and Anton Souslov[3]

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[2] *Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland*

[3] *School of Physics, Georgia Tech*

This talk will explore elastic and mechanical properties and mode structures of model periodic isostatic lattices, such as the square and kagome lattices, that are just on verge of mechanical instability [1]. It will focus particularly on the origin and nature of zero modes of these structures under both periodic (PBC) and free boundary conditions (FBC), and it will derive general conditions under which (a) the zero modes under the two boundary conditions are essentially identical and (b) under which zero modes do not appear in the periodic spectrum but do appear as surface waves in the free spectrum. In the former situation, lattices are generally in a type of critical state, and distortions away from that state give rise to surface modes under free boundary conditions whose degree of penetration into the bulk diverges at the critical state. This general phenomenon also occurs in sub-isostatic lattices like the honeycomb lattice [Fig.1(a)].

Consider N particles in d dimensions. In the absence of constraints or interactions, these particles have dN zero-energy translational modes. The addition of a central force spring or rigid strut between any two particle reduces the number of zero modes by one. Thus, if N_B springs are added, the expectation is that there would be $N_0 = dN - N_B$ zero modes, a result first noted by Maxwell [2]. This relation, however, does not take account of the possibility that the addition of a spring, rather than reducing the number of zero modes, merely strengthens the structure. In the latter case, the extra rigidity is signalled by the presence of a “state of self-stress" [3] in which springs can be put under positive or negative tension leaving forces on all particle equal to zero as depicted in the Fig. 1(b).

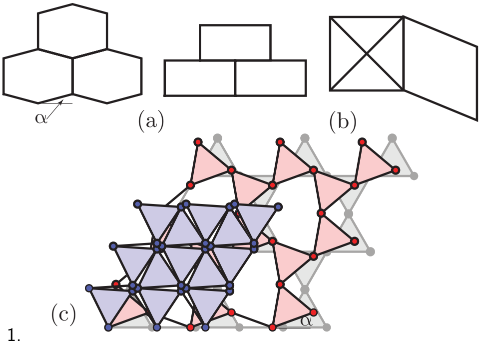

FIG. 1.
(a) Compressed honeycomb structures. The right-hand structure with $\alpha = 0$ has one state of self-stress per horizontal line.
(b) A frame with 6 sites and 9 bonds so that $dN - N_B = 3$. There is one internal zero mode in which the right-hand square is sheared and one state of self stress in the left-hand square.
(c) A series of kagome lattice formed by rotating triangles through an angle α. The $\alpha = 0$ lattice is the standard kagome lattice.

The relationship between zero modes and states of self stress can be couched in more mathematical terms with the aid of the equilibrium matrix $\mathbf{H}$, relating the vector $\mathbf{t}$ of of N_B bond tensions to the vector $\mathbf{f}$ of dN components of force: $\mathbf{H} \cdot \mathbf{t} = \mathbf{f}$, and the compatibility matrix $\mathbf{C} \equiv \mathbf{H}^T$, relating the vector $\mathbf{d}$ of dN particle displacements to the vector $\mathbf{e}$ of N_B spring extensions: $\mathbf{C} \cdot \mathbf{d} = \mathbf{e}$. The nullspace of $\mathbf{H}$ is spanned by the independent states of self stress, and its dimension S is the number of state of self stress; the nullspace of $\mathbf{C}$ of dimension N_0 is spanned by the set of independent displacements that leave spring lengths unchanged are are thus of zero energy. The rank-nullity theorem of linear algebra states that the $R + S = N_B$ and $R + N_0 = dN$ where R is the rank of both $\mathbf{H}$ and $\mathbf{C}$. Thus

$$N_0 = dN - N_B + S.$$

In periodic isostatic lattices there are exactly $2d$ neighbors per particle, and $N_B = dN$. Thus any zero modes under PBCs arise from states of self-stress, which are often, as in the case of the square and kagome lattices, associated with straight lines of bonds that traverse the sample. When a finite

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section with N sites of such a lattice is removed from the periodic one, there are no states of self stress, but there are of order $\sqrt{N}$ fewer bonds and of order $\sqrt{N}$ zero modes. Zero bulk modes under PBC survive as bulk zero modes under FBC. Periodic isostatic lattices, such as the twisted kagome lattices of Fig. 1(c), have only two states of self-stress and two associated zero modes corresponding to the two rigid translations under PBC. Under FBC, they must have of order $\sqrt{N}$ zero modes. They appear as zero-energy surface Rayleigh waves, which in the case of the twisted kagome lattice at long wavelength represent conformal distortions of the lattice. As the untwisted lattice is approached by reducing the twisting angle α, the penetration of surface modes into the bulk increases, finally diverging at the untwisted lattice. This talk will explore these properties of the kagome and other related lattices in detail.

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[3] C.R. Calladine, Intern. J. of Solids and Structures **14**, 161 (1978).

A2 **Rolf Schilling** **$09^{30} - 10^{00}$**

Spreading of localized excitations

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Studying the temporal evolution of a localized excitation two questions may arise. First, does a localized excitation spread completely or not, for time going to infinity? Second, if the spreading is incomplete does a critical excitation amplitude A_c exist such that the spreading is complete for $A < A_c$ and incomplete for $A > A_c$? In the latter case energy transport would become suppressed. For harmonic systems without quenched disorder W.R. Hamilton in 1841 already proved that the spreading is always complete.

For liquids, mode-coupling theory(MCT) [1] predicts that a localized density fluctuation does not spread completely for T below a critical temperature T_c . Here, we consider a solid which is decomposed into a subsystem of anharmonic d.o.f. $\{q_\alpha\}$ interacting bilinearly with the remaining d.o.f. $\{x_n\}$ taken as harmonic. For Newtonian dynamics we have shown [2] that a localized excitation converges to zero or to a localized time-periodic solution (LTPS). In presence of quenched disorder, additionally, convergence to weakly-chaotic solutions might occur.

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To quantify these predictions and to explore the existence of a critical amplitude A_c we have studied one of the simplest models, a chain of particles with harmonic nearest neighbor coupling, except for a single bond q_M with quartic anharmonicity. Eliminating the harmonic d.o.f. leads to the integral equation

$$q_M(t) = AJ_0(t) - \int_0^t dt' J_1(t-t') q_M^3(t') \qquad (1)$$

with $J_n(t)$ the Bessel function of order n and the initial conditions $q_M(0) = A$, $\dot{q}(0) = 0$. Its analytical discussion [3] proves the existence of $A_c > 0$ such that the relaxation time $\tau_{\mathrm{rel}}(A)$ is finite for $A < A_c$ and diverges at A_c. Consequently, there is complete spreading for $A < A_c$. For $A > A_c$ the initially localized excitation must converge to a LTPS [2] with amplitude $q_M^{\mathrm{env}}(A) > 0$. The numerical solution[3] of Eq.1 provides more insight into that kind of "ergodic-nonergodic" transition. q_M^{env} determined at a final time τ_i is presented in Figure 1. This figure gives strong evidence for a continuous transition at A_c. The numerical solution also allows to determine $\tau_{\mathrm{rel}}(A)$ for $A < A_c$ and a time $\tau_{\mathrm{mod}}(A) = 2\pi/\omega_{\mathrm{mod}}$ for $A > A_c$ (see Figure 2). Both time scales exhibit power law divergence with nontrivial exponents, analogous to MCT.

Since the control parameter A characterizes a nonequilibrium situation there can not exist a *static* length scale diverging at A_c. This is in variance with a recent prediction [4]. However, we have found a diverging *dynamic* length scale [5] for A approaching A_c from above

$$\xi(A) \sim (A - A_c)^{-\beta/2} \quad , \quad \beta > 1 \qquad (2)$$

On that scale the particles oscillate *cooperatively*. But no such dynamical length scale has been found yet for $A \to A_c$ from below.

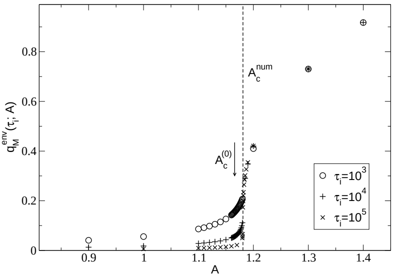

FIG. 1. Amplitude at times τ_i as a function of the initial excitation amplitude A .

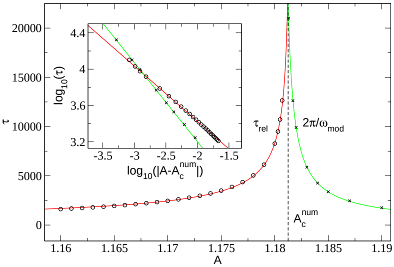

FIG. 2. Renormalized relaxation time τ_{rel}(circles) and modulation time $2\pi/\omega_{\mathrm{mod}}$ (crosses) as function of A. The solid lines represent power law fits of τ_{rel} and and $2\pi/\omega_{\mathrm{mod}}$ with exponents 0.61 and 0.87, respectively, which are supported by the log-log plots of the inset

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A3 **Kurt Binder** **$10^{00} - 10^{30}$**

Modeling transport in confined colloidal crystals in equilibrium and under compression and shear deformations

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Langevin Dynamics simulations are used to study a model for a two-dimensional colloidal crystal confined by corrugated parallel walls. Both the case when a perfect triangular lattice structure with $n = 30$ rows parallel to the walls fit into the crystalline strip is considered, and the case when by compression a mismatch is created. This may lead (at constant particle number) to a transition from n to $n - 1$ rows, accompanied by the formation of a soliton staircase pattern along the corrugated walls and a jumpwise decrease in the stress [1–4]. It is found that already in equilibrium at temperatures far below melting diffusion of the particles occurs. In addition to the standard vacancy interstitial mechanism also cooperative rotation of "rings" of 3 or 6 particles is found to occur. In the case of compressed crystals with soliton patterns the motion of solitons creates additional mobility [5].

When the corrugated walls are moved with a velocity v_{shear} in opposite directions, a nonlinear velocity profile $v(y)$ is created across the stripe. For small shear several rows along the walls are melted, while the central part of the stripe breaks up into large crystalline clusters, with somewhat misoriented lattice directions, slowly rearranging themselves and thus creating mobility in the flow direction. The temperature still stays essentially constant in the stripe. However, for strong shear the temperature gets enhanced near the walls, but only very few rows get disordered and mobile [6].

Acknowledgements: This research has been supported by the Deutsche Forschungsgemeinschaft, Sonderforschungsbereich TR6/C4.

[1] Y.-H. Chui, S. Sengupta, and K. Binder, EPL **83**, 58004 (2008)
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[3] Y.-H. Chui, S. Sengupta, I. K. Snook and K. Binder, J. Chem. Phys. **132**, 074701 (2010)
[4] D. Wilms. N. B. Wilding, and K. Binder, Phys. Rev. E**85**, 056703 (2012)
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[6] D. Wilms, P. Virnau, S. Sengupta, and K. Binder, preprint.

B1 **Vincent Krakoviack** $11^{00} - 11^{30}$

Mode-coupling theory, quenched randomness and self-generated disorder

Vincent Krakoviack[*]

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Using standard projection operator techniques, the mode-coupling theory (MCT) of the liquid-glass transition can be extended to deal with the slow dynamics of fluids evolving in statistically homogeneous random environments [1–5]. In this talk, we report on various aspects of this extension of MCT, which is in particular relevant for the study of the effects of confinement on glassforming liquids [6, 7].

We first review some generic structural properties of fluids in disordered environments, that result from the interplay between the two averages present in the problem, over thermal fluctuations and quenched disorder, respectively. We show how they can be incorporated into the projection operator derivation of MCT, leading to equations that pass a number of nontrivial consistency tests. These equations point towards a physical scenario in which two parallel mechanisms cooperate to slow down the dynamics.

We then present the different dynamical scenarios that are obtained when the theory is applied to simple model systems. The corresponding dynamical phase diagrams are computed, which show new and nontrivial transition patterns (see Fig. 1 for examples). In many cases, at least partial agreement is found with computer simulations [8–12] and other theoretical frameworks [13, 14], but spectacular disagreements can also appear [15, 16].

Finally, time permitting, we will show how variations on the theme of MCT and fluids in quenched-disordered environments can be used to contrast different qualitative pictures of (ideal) glass formation, where reference to some kind of self-generated (or self-induced) disorder is sometimes made.

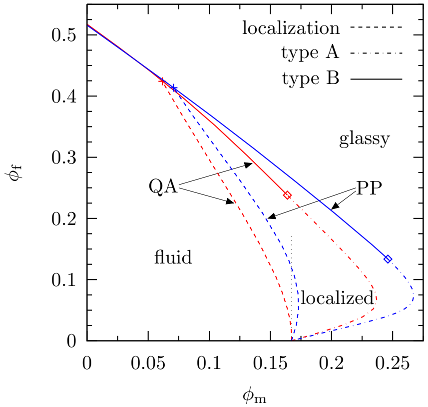

FIG. 1. Mode-coupling dynamical phase diagrams of the equisized hard-sphere quenched-annealed (QA) and partly pinned (PP) fluid-matrix models. ϕ_f and ϕ_m denote the volume fractions occupied by the fluid and matrix particles, respectively. From Ref. [5].

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B2 **Emanuela Del Gado** **$11^{30} - 12^{00}$**

Heterogeneous glasses and sustainable cement

Emanuela Del Gado*

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Novel breakthroughs in engineering materials, from cement to smart composites, depend crucially on understanding the microscopic physical processes controlling the formation of amorphous structures and leading to the arising of mechanical strength. I would like to discuss in particular how identifying the connection between long-range spatial correlations and heterogeneous dynamics in amorphous materials can give new indications for rationalizing their mechanical response.

In glassy alloys, the features of the potential energy landscape that control separately the microscopic dynamics of the liquid and the mechanical response of the amorphous solid closely intertwine upon approaching the glass transition. Identifying the parts of the potential energy surface undergoing non-affine rearrangements under deformation allowed us to unravel the long range spatial correlations underlying the cooperative microscopic dynamics observed in experiments and molecular dynamics simulations. Their correlations with the spatial distributions of localized soft modes suggest that such non-affinely re-arranging regions also play a role in the development of mechanical properties close to the glass transition [1–3]. Structure heterogeneity, as it is the case in real materials, can come into play in a way that is far from trivial, as recently shown by our studies of cooperative dynamical processes in re-structuring colloidal gel networks [4, 5]. Due to the long-range spatial correlations created by the mesoscale organization of the network, bond-breaking processes can induce non-local cooperative processes that are not present in non-restructuring networks. Starting from the soft parts of the network, where bond-breaking is more likely to occur, such events induce significant rearrangements of parts of the network structure further away.

I would also like to discuss how these concepts can be applied to investigate the development of structure and mechanical properties of the nano-scale, dense gel formed by calcium-silicate-hydrate (C-S-H), the primary hydration product of Portland cement [6]. It precipitates and solidifies during cement hydration, literally glueing together its different parts and it is responsible for its mechanics. We investigate how the competition between effective interactions and precipitation of hydrates determines a unique interplay between heterogeneous structure and dynamics, which leads to different microstructures and rheology. It has become increasingly clear that elucidating these points is crucial to develop new high performance and sustainable cementitious compounds [7].

We acknowledge the support of the Swiss National Science Foundation (Grant No. PP002 126483/1).

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B3 **Grzegorz Szamel** **$12^{00} - 12^{30}$**

Glassy dynamics of partially pinned fluids: an alternative mode-coupling approach

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We use a simple mode-coupling approach to investigate glassy dynamics of partially pinned fluid systems [1]. Our approach is different from the mode-coupling theory developed by Krakoviack [2]. In contrast to Krakoviack's theory, our approach predicts a random pinning glass transition scenario that is qualitatively the same as the scenario obtained using a mean-field analysis of the spherical p-spin model and a mean-field version of the random first-order transition theory [3]. We use our approach to calculate quantities which are often considered to be indicators of growing dynamic correlations and static point-to-set correlations [4]. We find that the so-called static overlap is dominated by the simple, low pinning fraction contribution. Thus, at least for randomly pinned fluid systems, only a careful quantitative analysis of simulation results can reveal genuine, many-body point-to-set correlations.

We gratefully acknowledge the support of NSF Grant CHE 0909676. GS thanks G. Biroli and C. Cammarota for a discussion that inspired this work.

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C1 Annette Zippelius $14^{00} - 14^{30}$

Cohesive Granular Fluids

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Cohesively interacting granular fluids have dramatically different mechanical pro- perties when compared to dry granular matter. In the dilute regime particles aggregate in a self-similar process which is analysed with event-driven simula- tions and scaling arguments. Even though granular fluids are inherently out of equilibrium, experiments on granular streams reveal many features which are fa- miliar from molecular fluids. An example is droplet formation in a freely falling stream of granular particles which cannot be explained by the Rayleigh-Plateau argument. We simulate a freely falling stream of granular particles and analyse the observed clustering instability in the framework of hydrodynamic equations, revealing that the stream is generically unstable. Initially a finite strain rate sta- bilizes the flow, but eventually all wave numbers become unstable for sufficiently long times. Since a freely falling stream corresponds to a nonstationary state, the growth rate of a perturbation with a given wavelength depends on the time, when the perturbation is introduced into the flow. We argue that in experiment these perturbations occur as spontaneous fluctuations, giving rise to a broad range of sizes and shapes of the observed clusters or droplets.

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C2 Claus Heussinger $14^{30} - 15^{00}$

Jamming and glassy dynamics in driven granular systems: "melting a glass by freezing"

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The jamming paradigm aims at providing a unified view for the elastic and rheological properties of materials as different as foams, emulsions, suspensions or granular media. Structurally, these systems can all be viewed as dense assemblies of particles, and the particle volume fraction ϕ plays the role of the coupling constant that tunes the distance to the jamming transition. Apart from the industrial relevance of these materials, there is also a fundamental theoretical interest in the (athermal) jamming transition: as a new paradigm for structural arrest its relation to the (thermal) glass transition, the characterization of common and distinguishing features, remain to be elucidated.

In this contribution we present simulation results for a driven granular system in its glassy phase at high volume fraction. We show evidence of a remelting transition into a fluid phase, which occurs by *reducing* the amplitude of the driving. This transition is accompanied by superdiffusion, cooperative particle motion and a negative differential diffusivity. We will highlight the special role played by frictional interactions, which help particles to escape their glassy cages. Such an effect is in striking contrast to what friction is expected to do: make particles stick to reduce their mobility.

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D1 **Eckhard Bartsch** 15^{00} – 15^{30}

Influence of particle softness and attraction range on gel and glass transitions in colloidal microgel suspensions with short-ranged depletion attraction

E. Bartsch,[1,2,*] S. Burger,[1,2] C. Stilke,[1,2] M. Wiemann,[1,2] and N. Willenbacher[3]

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The introduction of a short-ranged attraction to hard sphere-like colloidal particles, e.g. by addition of a non-adsorbing ("free") polymer, leads to a shift of the glass transition ϕ_g to higher volume fractions. At a particular attraction strength (= some polymer concentration) ϕ_g reaches a maximum value and the glass line then bends back, leading to a fluid pocket embedded between two types of glass states – the repulsive glass at low polymer concentration and the attractive glass at high polymer concentration. This phenomenon – called re-entrant glass transition – was first predicted by mode coupling theory (MCT) [1] and then verified by experiment [2, 3]. Remarkably, while this effect resulted in a shift of ϕ_g of about 10 % for hard sphere-like PMMA colloids [2], a more pronounced displacement of the glass transition of about 20 % was found for a binary mixture of slightly soft polystyrene (PS) microgel colloids [3], leading to fluid states up to volume fractions of 0.69 as determined by dynamic light scattering (DLS). This re-entry effect is not only of interest for fundamental science reasons. It may also have practical relevance as an alternative means to achieve freely flowing suspensions at highest particle concentrations.

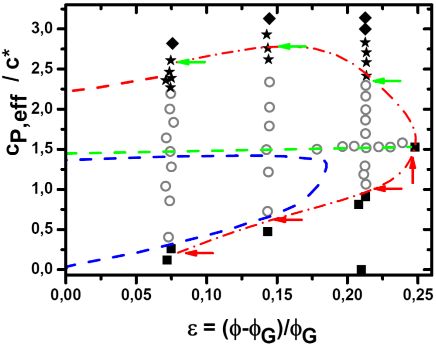

FIG. 1. Location of glass transition lines of 1:50 crosslinked microgel particles for two attraction ranges: $\delta = 0.059$ (red line), $\delta = 0.08$ (blue line). Symbols indicate the states for $\delta = 0.059$: ○ fluid, ■ repulsive glass, ◆ attractive glass, ⋆ clusters. $\phi_g = 0.58$.

To check whether the extraordinary shift of the glass transition is also reflected in the rheological behaviour we prepared similar binary colloid mixtures (size ratio $\Gamma = R_{small}/R_{large} = 0.72$) with free (PS) polymer ($\delta = R_{g,polymer}/R_{colloid} = 0.08$) at two different number ratios $N = N_{small}/N_{large} = 11$ and 2.5 and compared the dynamics as monitored by DLS and by steady shear rheology [4] for the same sample. We found that the locations of the glass transition in DLS and in rheology are identical within experimental error, thus verifying the presence of fluid states up to $\phi = 0.69$. No difference was observed between the different number ratios. MCT predicts that the fluid pocket of the re-entry region becomes more extended and shifts to even higher volume fractions on reducing the attraction range δ and that the attractive glass line merges with the gel line at low volume fractions [1, 5]. Thus, it was intriguing to systematically vary the polymer to colloid size ratio δ. We determined the kinetic arrest lines for $\delta = 0.055$, 0.068, 0.123, 0.163 and 0.3 over the volume fraction range $0.1 \leq \phi \leq 0.6$ by DLS. Correcting for free volume [6] and polymer non-ideality [7] we find that the gel line shifts to higher effective polymer concentration on reducing the attraction range δ. Intriguingly, the kinetic arrest occurs at almost constant contact potential over the whole volume fraction range for a given δ and the gel line appears to be continuous with the attractive glass line. Monitoring the re-entry region for $\delta = 0.059$ we find – as predicted by theory – a significantly broadened region of fluid states which extended up to a maximum volume fraction of ≈ 0.72. To elucidate the effect of particle "softness" we prepared more highly crosslinked PS microgel particles (1:10 = 1 crosslink per 10 monomer units as compared to previous 1:50 crosslink density) and studied the re-entry effect for a similar binary

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mixture of 1:10 microgel particles plus free polymer ($\delta = 0.08$). For these less soft particles we find a significantly reduced re-entry effect which is very similar to that of PMMA hard sphere colloids [8].

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D2 **Francesco Sciortino** **15^{30} – 16^{00}**

Re-entrant phase behavior of network fluids: A patchy particle model with temperature-dependent valence

F. Sciortino,[1,*] J. Russo,[1] L. Rovigatti,[1] J. M. Tavares,[2] P. I. C. Teixeira,[2] and M. M. Telo da Gama[2]
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In recent years the study of anisotropic interactions in simple fluids has led to an extraordinary progress in our understanding of the competition between self-assembly and phase separation. It is well known that, for particles interacting via isotropic potentials that comprise an excluded volume repulsion and a long-range attraction, condensation occurs when the energy drop associated with forming a high density liquid overcomes the concomitant loss of entropy. On the other hand, anisotropic interactions promote the aggregation of particles into self-assembled structures, such as chains, rings, and more complex clusters (e.g., micelles and vesicles). This aggregation process can compete with the clustering that drives condensation, giving rise to new phase behaviors.

In order to study the interplay between self-assembly and condensation systematically, a recent line of research has concentrated on the phase properties of patchy particles Patchy particles are particles whose surface is patterned so that they attract each other via discrete sites ('sticky spots') located on their surface. Among the advantages of patchy particles are their simplicity and the fact that the degree of anisotropy in the interactions can be fine-tuned by changing the number, type, size, and strength of the patches. However, the most important feature that makes patchy particles ideally suited for our investigation is the fact that both their thermodynamic and structural properties can be predicted with a high degree of precision using the thermodynamic first-order perturbation theory of Wertheim and the Flory-Stockmayer theory of polymerization. It is thus possible to study the criticality of patchy particles from a standard liquid state theory approach, without resorting to phenomenological theories.

In this communication we discuss[1, 2] a model consisting of particles with dissimilar bonding sites (patches), which exhibits self-assembly into chains connected by Y-junctions, and investigate its phase behavior by both simulations and theory. We show that, as the energy cost of forming Y-junctions increases, the extent of the liquid-vapor coexistence region at lower temperatures and densities is reduced. The phase diagram thus acquires a characteristic pinched shape in which the liquid branch density decreases as the temperature is lowered. To our knowledge, this is the first model in which the predicted topological phase transition between a fluid composed of short chains and a fluid rich in Y-junctions[3] is actually observed. Above a certain threshold for the branching energy, condensation ceases to exist because the entropy gain of forming Y-junctions can no longer offset their energy cost. We also show that the properties of these phase diagrams can be understood in terms of a temperature-dependent effective valence of the patchy particles. Connections with the dipolar hard-sphere model will be discussed[4].

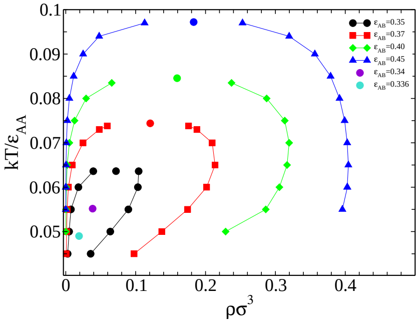

FIG. 1. Numerical estimates of the phase diagram of particles with dissimilar bonding sites, forming chains and Y-junctions, for different values of the explored parameters.

The Rome authors acknowledge support from ERC-PATCHYCOLLOIDS

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E1 Andreas Bausch $16^{30} - 17^{00}$

Cytoskeletal pattern formation: Self organization of driven filaments

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Living cells rely on the self organization mechanisms of cytoskeleton to adapt to their requirements. Especially in processes such as cell division, intracellular transport or cellular motility the controlled self assembly to well defined structures, which still allow a dynamic reorganization on different time scales are of outstanding importance. Thereby, the intricate interplay of cytoskeletal filaments, crosslinking proteins and molecular motors a central role. One important and promising strategy to identify the underlying governing principles is to quantify the physical process in model systems mimicking the functional units of living cells. Here I will present in vitro minimal model systems consisting of actin filaments, crosslinking molecules and myosin II exhibiting collective long range order and dynamics. I will discuss how a balance of local force exertion, alignment interactions, crosslinking and hydrodynamics affect the evolving dynamic structures.

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E2 **Hartmut Löwen** 17^{00} – 17^{30}

Transport in strongly interacting active colloids

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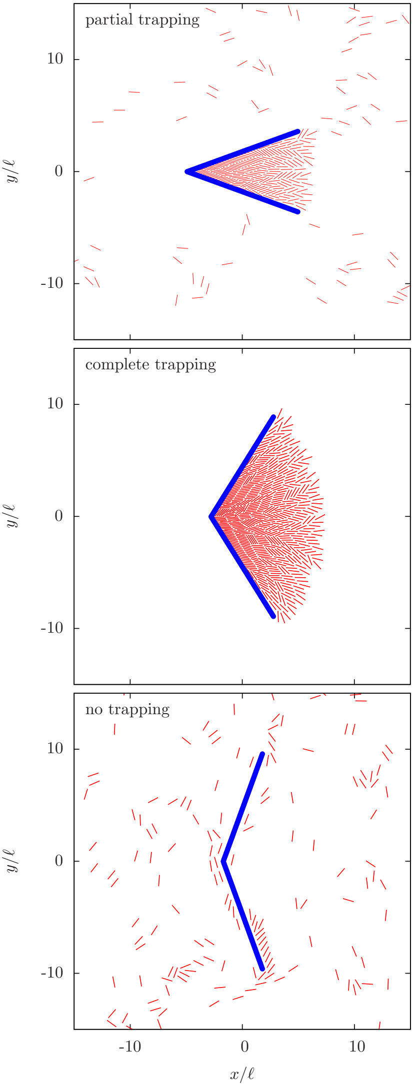
We explore the dynamics and transport properties of strongly interacting active colloidal particles by computer simulation and dynamical density functional theory. Brownian dynamics simulations are used to study the nonequilibrium dynamics of concentrated self-propelled rods which are interacting via a Yukawa segment model.

In a linear channel, transient hedgehog-clustering at the system boundaries is found [1]. An wedge-like confinement is shown to be a very efficient trap for active particles. Simulation snapshots corresponding to partial, complete and no trapping at different opening angles are shown in Fig. 1 [2]. In the two-dimensional bulk, anomalous turbulence emerges [3] in agreement with recent experimental data on bacterial motion [4].

Finally we study the freezing transition for very dense self-propelled particles and find significant differences to equilibrium freezing [5]. Simulation data are compared to a recent field-theoretical approaches of freezing based on the phase-field-crystal model which is extended towards active systems.



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Thursday

09:00 – 10:30 Complex Rheology

Chair: Walter Schirmacher

F1	**Jürgen Horbach**	*Non-linear active micro-rheology in glass-forming soft-sphere mixtures*
F2	**Stefan Egelhaaf**	*Concentrated colloidal suspensions under time-dependent shear*
F3	**Matthias Fuchs**	*History dependence of the nonlinear response of colloidal glasses*

10:30 – 11:00 Coffee break

11:00 – 12:30 Fast Dynamics

Chair: Robert Pick

G1	**Peter Lunkenheimer**	*Fast dynamics of glassforming liquids*
G2	**Ernst Rößler**	*Is there a link between high- and low-temperature dynamics in molecular liquids?*
G3	**Walter Schirmacher**	*Elastic heterogeneities in glasses and rigidity percolation: Revival of the F1 model*

12:30 – 14:00 Lunch break

14:00 – 15:30 Glass Transition

Chair: Vincent Krakoviack

H1	**Walter Kob**	*Equilibrium properties of glass-formers at the Kauzmann temperature*
H2	**Angel Moreno**	*Slow Dynamics in Polymer Melts: The Role of Intramolecular Barriers*
H3	**Francesco Zamponi**	*Glass transition of hard spheres in dimension from three to thirteen*

15:30 – 16:00 Coffee break

16:00 – 17:30 Diffusion

Chair: Winfried Petry

I1	**Andreas Meyer**	*On the relation of self diffusion and viscosity in dense liquids: New experimental results from electrostatic levitation*
I2	**Jörg Baschnagel**	*On the Anomalous Diffusion of a Polymer Chain in an Unentangled Melt*
I3	**Luca Cipelletti**	*Supradiffusive dynamics: from metallic glasses to actin networks*

19:30 – 23:00 Conference Dinner

F1 Jürgen Horbach $09^{00} - 09^{30}$

Non-linear active micro-rheology in glass-forming soft-sphere mixtures

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In active micro-rheology, the response of a tagged particle to an external force f is investigated. The steady-state motion of the tagged particle is characterized by an average constant velocity v that is related to f by a friction coefficient ξ via $\xi = f/v$. When the force f is sufficiently weak, the steady-state motion of the particle follows linear response theory which predicts a simple relationship between the equilibrium diffusion constant D of the tagged particle and the friction coefficient, $D\xi = k_B T$ (with k_B the Boltzmann constant and T the temperature). In glass-forming liquids relatively small forces f suffice to observe a non-linear response of the pulled particle. This has been shown in recent micro-rheological experimental studies of colloidal systems as well as simulation and mode-coupling theory (MCT) (see Ref. [1, 2] and references therein).

In this talk, results of molecular dynamics (MD) computer simulations of a simple glass-forming soft-sphere model are presented to reveal the non-linear single-particle response to a constant force. In the non-linear regime, the diffusion dynamics of the pulled particle is anisotropic. While the diffusion coefficient perpendicular to the force can be mapped onto the equilibrium dynamics in terms of an effective temperature, parallel to the force the "drift-corrected" mean-squared displacement (MSD) shows a superlinear behavior in the long-time limit (superdiffusion) provided that this long-time regime is much shorter than the typical time scale required for rearrangements in the surroundings of the pulled particle. We show that the latter superdiffusive behavior is not caused by the hydrodynamic backflow of the pulled particle. It associated with a cage-to-cage hopping and a broad distribution of waiting times in the cage; these properties are also seen in directed walks among traps with a broad release time distribution where the MSD may also display a superlinear behavior in the long-time limit [3].

Below the glass transition, a steady state motion of the pulled particle is only observed if the applied force is larger than a threshold force f_{th}. According to a schematic MCT model, a dynamic nonequilibrium delocalization transition occurs at f_{th} [2]. We discuss to what extent signatures of this transition are seen in our MD simulation.

The authors acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG), Projects No. SFB TR 6/A5 and No. FOR 1394/P8. Computer time at the NIC Jülich is gratefully acknowledged.

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F2 **Stefan Egelhaaf** **$09^{30} - 10^{00}$**

Concentrated colloidal suspensions under time-dependent shear

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The effect of time-dependent shear on concentrated and glassy hard-sphere suspensions is experimentally investigated and the results compared to theoretical and simulation predictions [1–3]. The rheological response to increasing strain (at constant strain rate) is characterized by a stress overshoot before steady-state flow is established. Using confocal microscopy, we relate this macroscopic behaviour to the microscopic structure and dynamics under the application of shear. The dynamics show a super-diffusive regime during the transition from in-cage to out-of-cage motion. At the same time, the shear-induced structural anisotropy is maximal. The degree of anisotropy and the magnitude of the overshoot is controlled by the Peclet number and the available free volume, which determine the ability of caged particles to relax deformations through Brownian motion. Structural anisotropy is still present in the steady-state of shear. After cessation of shear, the deformed cages result in an incomplete stress relaxation and a different localization length compared to the quiescent state. Our experimental results are compared to recent simulations and theoretical predictions [4, 5].

We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG) within the SFB-TR6 and FOR 1394.

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F3 **Matthias Fuchs** **$10^{00} - 10^{30}$**

History dependence of the nonlinear response of colloidal glass

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Glass is an isotropic solid and thus it appears very natural to describe it in terms of classical elasticity theory. Fluctuations of strain and of the other coarse-grained hydrodynamic fields like density and momentum density then should obey the framework of (time-dependent) linear response theory based on equilibrium statistical mechanics.

In this talk I will discuss different approaches, one of them based on mode coupling theory, which consider glass as a quasi-equilibrium solid and obtain elastic constants, phonon dispersion relations, and strain field from microscopic starting points. As glass is amorphous, the necessary evaluation of a strain field is not obvious. It requires to define particle displacements and average sites microscopically, even though no periodic lattice exists and long-ranged order appears lacking. Interest in these approaches arises from recent confocal or video microscopy studies of colloidal glass, which could measure the elasticity of amorphous solids from the particle trajectories [1]. The nonlinear response of individual particles, frozen in the glass, to strong external forces can then also be considered [2].

Yet, glass is a metastable state and depends on the history of its preparation. Extending mode coupling theory to capture the nonlinear response of glass under arbitrary time-dependent deformations [3], the dependence of the quiescent glass state on its shear history can be explored. Glass formed from the fluidized driven state keeps non-relaxed internal stresses which bear the signature of the preparation history and can severely influence the mechanical performance of the glass. Single particle motion detects their spatial correlations. I will present confocal microscopy data, rheological measurements, computer simulations, and schematic model [4] calculations within MCT which capture the dependence of the glassy state on its shear flow in the (infinite) past. The residual stresses and the length-scale of particle-hindrance in the mean-squared displacement increase with decreasing shear-rate.

I acknowledge crucial contributions to the reviewed work by M. Ballauff, J.M. Brader, F. Ebert, S.U. Egelhaaf, C. Harrer, J. Horbach, C.L. Klix, N. Koumakis, M. Krüger, M. Laurati, K. Mutch, G. Petekidis, A. M. Puertas, M. Siebenbürger, Th. Voigtmann, F. Weysser, and J. Zausch.

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G1 **Peter Lunkenheimer** $11^{00} - 11^{30}$

Fast dynamics of glassforming liquids

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In broadband dielectric loss spectra of glass forming materials, a number of different dynamic processes is revealed leading to a variety of spectral features like peaks, power laws, or minima that can arise in the whole accessible range from µHz to THz [1–3]. Except for the so-called α peak, which is mirroring the structural relaxation processes driving the glassy freezing at the glass transition temperature, the microscopic origin of the other spectral features is still controversially discussed. Understanding those processes seems to be a prerequisite for achieving a deeper insight into the mechanisms of the glass transition and the glassy state of matter in general. Especially, it seems clear nowadays that the different spectral features are closely interrelated and cannot be described independently.

In the present talk, I provide broadband spectra of a variety of glass formers extending up to the boson peak region. Of special interest are the result on glycerol, whose dielectric response is systematically modified by the addition of ions (Fig. 1). It is well known that dissolving salts like, e.g., LiCl, in glycerol leads to strong shifts of the α-relaxation peaks [4, 5]. However, almost nothing is known about the behavior of the faster processes like excess wing, fast beta process, and boson peak, which all are observed in pure glycerol [2, 6]. For example, according to mode coupling theory, which well describes various dynamic properties of pure glycerol [7–10], the temperature dependences of such different quantities as the alpha-relaxation rate (in the mHz to GHz range) and the frequency of the loss minimum (10 - 100 GHz), are predicted to be closely correlated. These correlations are discussed in detail, also including results on other glass formers.

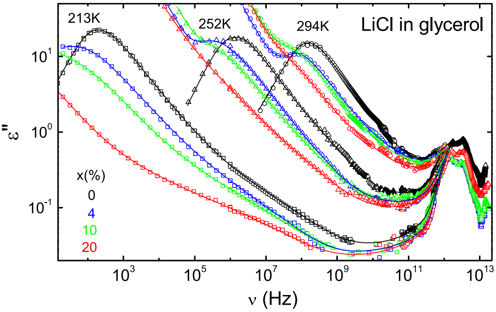

FIG. 1. Comparison of broadband dielectric loss spectra of glycerol-salt mixtures with various LiCl concentrations, shown for three typical temperatures. For better readability, in the boson-peak region ($\nu > 1$ THz) the results are shown for 252 K, only. The lines are guides to the eyes.

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G2 **Ernst Rößler** **$11^{30} - 12^{00}$**

Is there a link between high- and low-temperature dynamics in molecular liquids?

N. Petzold, B. Schmidtke, R. Kahlau, and E. A. Roessler*

Experimentalphysik II, Universitaet Bayreuth

Although broadly studied close to T_g molecular glass formers are not well investigated in the high-temperature regime above their melting point T_m. Most experiments are restricted to time scales above $10^{-9}s$ ignoring a large temperature range until the high-temperature limit $\tau_\infty \cong 10^{-12}s$ is reached. For example, dielectric spectroscopy (DS) probing molecular reorientation usually does not cover frequencies above few GHz. Reorientational correlation times down to $10^{-12}s$ are easily available by dynamic light scattering (LS) using tandem-Fabry-Perot interferometer (TFPI) and double monochromator (DM). Combining such techniques with state-of-the-art photon correlation spectroscopy (PCS) broad band susceptibility spectra comparable with those of DS become accessible [1].

We measured depolarized LS spectra of a series of molecular liquids up to 440 K concentrating on low-T_g systems for which the high-temperature limit is indeed reached. It turns out that typical "glassy dynamics" characterized by two-step correlation function, stretched long-time decay and frequency-temperature superposition set in well above T_m. Except for an ever increasing time constant τ_α no significant further change is observed in the correlation function while cooling from T_m down to T_g (fig. 1). In particular, no change of the amplitude of the α-process is found. However, subtle effects are recognized when susceptibility spectra are analyzed. Here, an anomaly of the relaxation strength $1-f$ of the fast dynamics is found (inset fig. 1) being a reorientational analogue of the anomaly of the Debye-Waller factor forecast by mode coupling theory. The effect is such small that it is not recognized in the plateau of the correlation function in fig. 1. The crossover may be linked to the appearance of the so-called excess wing which we identified also in the PCS data (fig. 2) as before by DS. Comparing the stretching of the α-process as measured by LS and DS we find it probe dependent without systematic correlation. Many glass former show a Johari-Goldstein β-process which is well identified by DS, NMR and mechanical relaxation. However, it does not show up in PCS experiments (inset fig. 2), a phenomenon not yet understood.

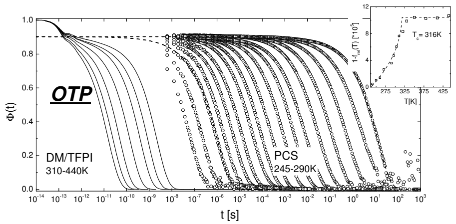

FIG. 1. step response $\Phi(t)$ of o-terphenyl measured by different LS techniques; $T_m = 332K$,
inset: relaxation strength of fast dynamics $1-f$ extracted from DM/TFPI-spectra

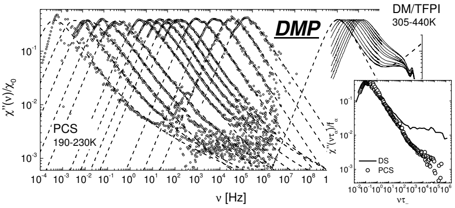

FIG. 2. normalized LS susceptibility spectra $\chi''(\nu)/f_\alpha$ of the glass former dimethyl phthalate,
inset: comparison PCS vs DS spectrum at $T = 198K$

Concerning the time constants τ_α we cover temperatures from boiling point down to T_g. Describing the dynamics in terms of an activation energy $E(T)$, we distinguish a high-temperature regime characterized by an Arrhenius law with a constant activation energy E_∞ and a low-temperature regime for which $E_{coop}(T) \equiv E(T) - E_\infty$ increases while cooling. T_g and E_∞ exhibit some correlation and a two-parameter scaling is introduced, specifically $E_{coop}(T)/E_\infty \propto exp\,[-\lambda(T/T_A - 1)]$, where λ is the generalized fragility and T_A a reference temperature proportional to E_∞. Thus, a single interaction

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parameter E_∞ describing the high-temperature regime together with λ controls the temperature dependence of low-temperature cooperative dynamics. A master curve results when the reduced energy $E_{coop}(T)/E_\infty$ is plotted vs reduced temperature (fig. 3). The experimental findings suggest that T_A is close to T_c of MCT.

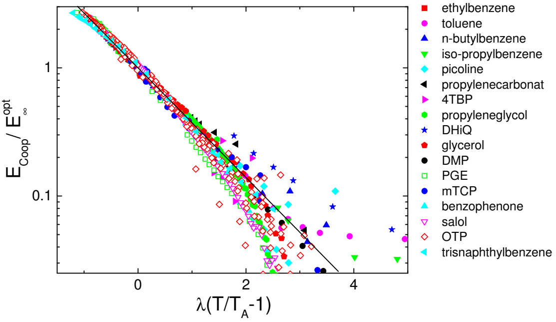

FIG. 3. master curve of the reduced activation energy as a function of rescaled temperature with $T_A \sim 0.11 E_\infty$; E_∞ high-temperature activation energy, λ generalized fragility

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G3 Walter Schirmacher $12^{00} - 12^{30}$

Elastic heterogeneities in glasses and rigidity percolation: Revival of the F1 model

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A theory for the vibrational properties of a disordered solid is presented based on the model assumption of spatially fluctuating shear moduli ("elastic heterogeneity"). The model is solved by field-theoretical techniques yielding self-consistent mean-field equations for the disorder-induced elastic self-energy (Self-consistent born approximation, SCBA [1, 2]). The theory successfully describes the appearance of a low-frequency enhancement of the vibrational spectrum ("boson peak") and the corresponding acoustic anomalies. The only adjustable parameter is the disorder parameter γ, which is proportional to the mean-square fluctuations of the shear modulus. As the theory is based on a Gaussian distribution of shear moduli there exists a critical value of γ, γ_c, beyond which the system is unstable.

Results of a very-large scale simulation of the vibrational dynamics of a soft-sphere glass (Repulsive part of a Lennard-Jones potential) are presented. >From the current-current fluctuation spectra the density of states, the anomalous sound dispersion and attenuation of the longitudinal and transverse excitations are extracted. They agree very well with the SCBA results with $\gamma - \gamma_c = 0.008$.

If a small anharmonic damping part is included in the SCBA equations [3], the theory near γ_c can be formally mapped [4] onto the so-called F_1 schematic model [5] of Götze's mode-coupling theory [6]. Near critically a frequency-fractal exponent of 1.5 is predicted both for the sound attenuation coefficient as well as for the vibrational density of states. Such an anomalous frequency dependence is, indeed, observed in the simulation data at low frequency. The temperature dependence of this contribution points to its anharmonic origin.

However, whithin our theory the anomalous frequency dependence is only obtained right at marginal instability, where no boson peak is predicted, as the latter describes a transition from a Debye spectrum to a disorder-induced one. From these findings we conclude that within the simulated glass soft regions with $\gamma \approx \gamma_c$ exists, surrounded by regions with $\gamma < \gamma_c$. Assuming a fraction of 10 % of marginally-stable regions gives very good fits to the data (see Fig. 1).

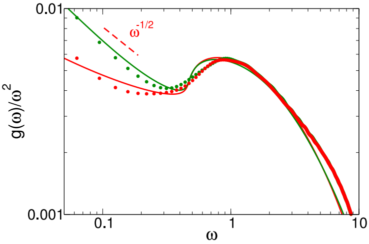

FIG. 1. "Reduced" density of states $g(\omega)/\omega^2$ of the simulated soft-sphere glass for two different temperatures (in Lennard-Jones units). The straight lines are the results of the SCBA calculations with an anharmonic damping term included and with the model assumtion of the existence of 10 % marginally-stable regions ($\gamma - \gamma_c = 10^{-5}$). In the remaining regions we put $\gamma - \gamma_c = 0.008$.

As such anomalous low-frequency vibrational spectra are also found experimentally in several glasses we conclude that generically glasses contain marginally stable regions in a heterogeneous way.

Possible relations to the low-temperature regime of the glass-transition scenario are discussed. In particular we try to explore connections to the non-thermal pathway of the so-called jamming transition, which is related to a percolation transition of rigidity. Both in simulational data presented in the literature and in our generalized SCBA model the rigidity is finite at the marginal-stability point, i.e. the rigidity-percolation transition appears to be a first-order one.

[1] W. Schirmacher, Europhysics Letters, **73**, 892 (2006).
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H1 **Walter Kob** **$14^{00} - 14^{30}$**

Equilibrium properties of glass-formers at the Kauzmann temperature

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The Kauzmann temperature T_K is one of the fundamental temperatures of glass-forming systems. However, since the relaxation times become very large already well above T_K, the properties of glass-formers around T_K cannot be studied *in equilibrium.* Recently it has been argued that, by randomly pinning particles, the properties of the liquid can be probed even close to T_K [1, 2]. In this talk I will present the results of computer simulations in which we use this novel approach. We find evidence that at T_K the system does indeed undergo a first-order like transition to an ideal glass state.

Part of this work has been supported by the Institut Universitaire de France.

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H2 Angel J. Moreno 14^{30} – 15^{00}

Slow Dynamics in Polymer Melts: The Role of Intramolecular Barriers

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[3] *Dipartimento di Fisica and CNR-ISC, Università di Roma La Sapienza, Roma, Italy*
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By means of simulations and solution of the Mode Coupling Theory (MCT), we investigate the role of the intramolecular barriers on several dynamic aspects of non-entangled polymers. The simulations are performed for a generic model of bead-spring chains with intramolecular barriers (bending and torsion potentials). The simulations cover a broad range of barrier strength between the limits of flexible and stiff chains. The investigated dynamic range extends from the caging regime characteristic of glass-formers to the relaxation of the chain Rouse modes. Solutions of MCT for the structural relaxation reproduce qualitative trends of simulations for weak and moderate barriers. However a progressive discrepancy is revealed as the limit of stiff chains is approached (see Fig.1). This disagreement does not seem related with dynamic heterogeneities, which indeed are not enhanced by increasing barrier strength [2]. It is not connected either with the breakdown of the convolution approximation for three-point static correlations, which retains its validity for stiff chains [2]. These findings suggest the need of an improvement of MCT for polymer melts. Concerning the relaxation of the chain degrees of freedom, MCT provides a microscopic basis for time scales from chain reorientation down to the caging regime. It rationalizes, from first principles, the observed deviations from the Rouse model on increasing the barrier strength. These include anomalous scaling of relaxation times, long-time plateaux, and non-monotonous wavelength dependence of the Rouse mode correlators (see Fig.2 for a representative example) [2].

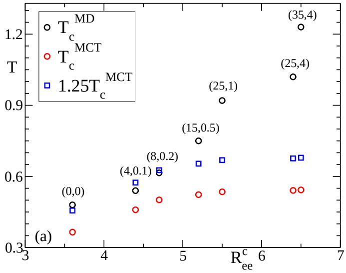

FIG. 1. Critical temperature T_c as a function of the end-to-end radius R^c_{ee} (measured at T^{MD}_c). The theoretical values T^{MCT}_c are compared with the simulation values T^{MD}_c. The respective values of the bending and torsional strength (K_B, K_T) —see [2] for model details— are indicated on top of each symbol.

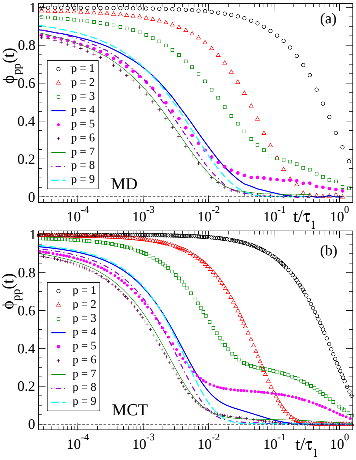

FIG. 2. Normalized Rouse mode correlators $\Phi_{pp}(t)$ for stiff chains with $(K_B, K_T) = (35, 4)$. Panel (a): simulation results at $T = 1.48$. Panel (b): MCT numerical solutions at $T = 0.63$. In both panels, the absolute time is rescaled by the relaxation time τ_1 of the $p = 1$ mode.

[1] M. Bernabei, A.J. Moreno and J. Colmenero, J. Chem. Phys. 131 (2009) 204502.
[2] M. Bernabei, A.J. Moreno, E. Zaccarelli, F. Sciortino and J. Colmenero, J. Chem. Phys. 134 (2011) 024523.

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H3 **Francesco Zamponi** **$15^{00} - 15^{30}$**

Glass transition of hard spheres in dimension from three to thirteen

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The glass problem is notoriously hard and controversial. Even at the mean-field level, little is agreed about how a fluid turns sluggish while exhibiting but unremarkable structural changes. It is clear, however, that the process involves self-caging, which provides an order parameter for the transition.

We studied numerically the glass transition of hard spheres in dimension $d = 3 \cdots 13$ [1]. The advantage of this study is that when dimension increases, the system approaches its mean field limit, in which the problem should simplify. Moreover, crystallization is strongly suppressed for $d > 3$ which allows us to study a monodisperse system without having to care about the crystal. One could expect in particular that self-consistent static and dynamic description of the glass transition, such as mode-coupling theory, density functional theory, and replica theory, should become more accurate in larger dimensions.

However, our results are not consistent with predictions from mode-coupling theory, and only partially consistent with replica theory. In particular, it is broadly assumed that the caging order parameter (the long time limit of the self Van Hove function in the glass) should have a Gaussian shape in the mean-field limit. Here we show that this ansatz does not hold: the cage keeps a non-trivial form in all dimensions. Quantitative descriptions of the glass transition, such as mode-coupling theory, density functional theory, and replica theory, all fail to describe the shape of the cage.

Although the mean-field random first-order transition scenario of the glass transition is qualitatively supported by our data and non-mean-field corrections are found to remain small on decreasing d, reconsideration of its implementation is needed for it to result in a coherent description of experimental observations.

We thank J. Kurchan and R. Schilling for stimulating discussions. P.C. acknowledges NSF support No. DMR-1055586.

[1] P.Charbonneau, A.Ikeda, G.Parisi, F.Zamponi, `arXiv:1205.4057`.

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I1 **Andreas Meyer** **$16^{00} – 16^{30}$**

On the relation between self diffusion and viscosity in dense liquids: New experimental results from Electrostatic Levitation

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The dynamics in fluids is governed by two intimately related properties: viscosity and atomic diffusion. While the first describes macroscopic transport of momentum by collective motion of the particles, the latter describes single particle diffusive transport. A common relation, which is often taken for granted in order to calculate required diffusion coefficients of atoms or molecules in a liquid from the viscosity, or vice versa, is the Stokes-Einstein relation:

$$D\eta = \frac{k_B T}{6\pi r_{\mathrm{H}}}. \tag{1}$$

In Eq. (1), η is the viscosity of the solvent, D diffusion coefficient, r_{H} its hydrodynamic radius, T is the absolute temperature, and $k_{\mathrm{B}} = 1.38\times10^{-23}$J/K is the Boltzmann constant.

The Stokes-Einstein relation was derived in order to study the diffusive motion of a mesoscopic sphere in a viscous medium. However, when the diffusing objects are of atomistic size, deviations of D and η from the Stokes-Einstein behavior can be observed.

From an experimental point of view, a direct proof of Eq. (1) is still very difficult due to the lack of reliable experimental data, especially of the transport coefficients D and η. The accurate measurement of diffusion data, using long capillary methods, is subject to large errors due to additional transport of mass by buoyancy driven flow effects [1, 2]. Pollution of the sample from chemical reactions with the container walls complicates the measurement of both properties. In order to check Eq. (1), measurements need to be carried out over a sufficiently large temperature range in which T changes by a factor of 1.5 - 2. This includes high temperatures favoring convection and chemical reactivity. With the development of advanced containerless processing techniques, such as electrostatic levitation (ESL), we are now in a position to master these challenges.

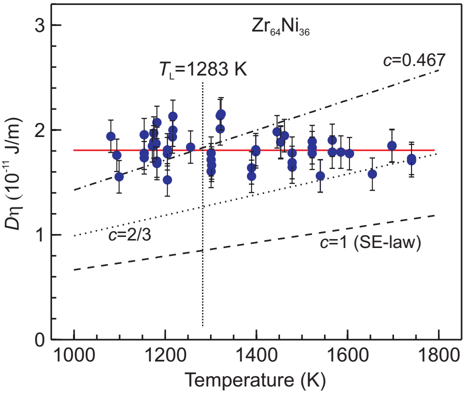

FIG. 1. $D_{\mathrm{Ni}} \cdot \eta$ versus temperature (symbols). In order to guide the eye, a linear fit to data is also shown (solid line). The dashed and dotted lines correspond to the Stokes-Einstein relation, Eq. (1), with different choices of the hydrodynmaic radius $r_{\mathrm{H}} = c r_{\mathrm{Ni}}$.

Using ESL, we carried out quasielastic neutron scattering (QNS) experiments and determined accurate Ni-self diffusion coefficients, D_{Ni}, in liquid $Zr_{64}Ni_{36}$and bulk glass-forming ZrTiNiCuBe alloys. These data were measured over a broad temperature range from 1000 K to 1700 K. Viscosity of these liquids were also measured via the oscillating drop technique in ESL over a broad temperature range: With these results for a dense glass forming system, the relation of viscous flow and diffusion of mass could be checked in unequaled detail.

Our data show that $D\eta = const$ for the entire temperature range (Fig. citefig1) contradicting the Stokes-Einstein relation. According to Mode-Coupling-Theory (MCT), the dynamics in a liquid is strongly coupled when the particle density is large. This leads to a freezing of the atomic motion when a critical temperature T_c is approached upon cooling. In this case, the diffusion coefficient D and the

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inverse of the viscosity, η^{-1}, are proportional to the same scaling law. Hence, when $T \to T_\mathrm{c}$, $D\eta = const$ is asymptotically obtained. Our results have been obtained at temperatures well above T_c. Apparently, possible deviations from the MCT scaling behaviour are similar with respect to temperature for both mass transport coefficients. Whether, this is also valid for other glass forming liquids and also less dense liquids is subject of ongoing research.

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I2 **Jörg Baschnagel** **$16^{30} - 17^{00}$**

On the Anomalous Diffusion of a Polymer Chain in an Unentangled Melt

J. Farago, H. Meyer, A. N. Semenov, J. P. Wittmer, A. Johner and J. Baschnagel*

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The dynamics of polymer chains in unentangled melts is commonly described by the classical Rouse model, a single-chain approach assuming Fickian diffusion dynamics of the monomers and neglecting excluded-volume interactions of chain segments. However, various experimental and simulation studies show that certain dynamical phenomena in unentangled melts cannot be explained by the Rouse theory. One of the puzzling observations is the anomalous diffusion of the center-of-mass (CM) of a polymer chain for times $t < t_N$, where $t_N \propto N^2$ is the Rouse time of a polymer consisting of N monomers.

Previous attemps to explain this observation have employed the coupling of the CM motion to the density fluctuations of the melt. We reanalyze this approach in the framework of a density-based mode-coupling theory (dMCT) and find a partial success [1]: The theory accounts for the anomalous motion by yielding a negative power-law tail for the CM velocity autocorrelation function (CM VAF), $C_\mathrm{cm}(t) \propto -N^{-1}t^{-5/4}$. This prediction is in good agreement with simulations utilizing a Langevin or Monte-Carlo dynamics. However, it appears that the magnitude of the effect is (strongly) underestimated by the theory.

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This suggests that another (or additional) mechanism could be operational. In the classical theory on polymer dynamics the friction force on a monomer results from the difference of its velocity with respect to that of the surrounding polymer matrix, which can itself be in motion. We find that such a collective continuous ('hydrodynamic') flow is indeed important [2–4]: It provides the dominant contribution to the anomalous CM dynamics, while the effect of density fluctuations analyzed by the dMCT appears to be subdominant.

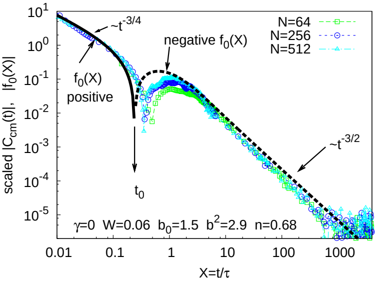

FIG. 1. Comparison between the theoretical scaling function $|f_0(X)|$ (solid line: positive part, dashed line: negative part) and the simulation data for $N = 64, 256, 512$ (squares, circles, and triangles, respectively), for a polymer model with crossable chains (to avoid entanglements) under momentum conserving dynamics. The simulation curves present $nb^3N^{3/2}\pi|C_{\text{cm}}(t)|/(\sqrt{24}v_T^2)$ as a function of t/τ. Here n is the number density of monomers, b the effective bond length, v_T the thermal velocity, and $\tau = (\pi/18)^{1/3}(Nb^2\sqrt{W}/v_T^2)^{2/3}$ with W being the monomer friction constant. The vertical arrow indicates the predicted sign inversion at $X \simeq 0.24$. Figure taken from Ref. [2].

Three complementary approaches have been devised to support this conclusion: (i) a version of the MCT coupling the CM motion to the collective flow (hydrodynamic interactions) [2], (ii) an approach based on hydrodynamic interactions, appropriately generalized to take into account viscoelastic hydrodynamic interactions (VHI) inherent in polymer melts [3], and (iii) a further derivation using a fluctuating hydrodynamics approach [4].

One result of this work is presented in Fig. 1. The figure compares simulation results (symbols) for polymer melts with momentum-conserving dynamics to the theoretical predictions (lines). At late times we find that the CM VAF decays as a power-law, $C_{\text{cm}}(t) \propto -N^{-1/2}t^{-3/2}$, resulting from the coupling to the hydrodynamic flow to the viscoelasticity of the melt. In this theoretical framework, we also revisit the situation of non momentum-conserving dynamics, as realized in Monte-Carlo or Langevin simulations. We find that the loss of the conservation law modifies the velocity relaxation of the CM, although the viscoelastic hydrodynamic effects still make a strong contribution to the CM motion. Interestingly in a certain time regime, we recover $C_{\text{cm}}(t) \propto -N^{-1}t^{-5/4}$, i.e., the behavior predicted by the dMCT approach, albeit with a much larger prefactor. This could imply that in cases, where the monomer friction is high, like in Monte-Carlo simulations [5], a weighted combination of both mechanisms—dMCT and VHI—must be employed for a quantitative description.

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I3 **Luca Cipelletti** **$17^{00} - 17^{30}$**

Supradiffusive dynamics: from metallic glasses to actin networks

Luca Cipelletti[1, 2, *]

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Very recent experimental work by B. Ruta *et al.* [1] shows that structural relaxation in metallic glass, as probed by X-photon correlation spectroscopy, exhibits a transition from diffusive behavior to an anomalous regime as temperature is lowered below the glass transition temperature, T_g. Above T_g, the intermediate scattering function decays as a stretched exponential function, $f(q,\tau) \sim \exp[-(\tau/\tau_\alpha)^p]$ with $p < 1$, as often observed in glassy systems. By contrast, içn the anomalous regime below T_g, p is larger than one, indicating a steeper-than-exponential decay that is incompatible with diffusive motion.

Such a 'compressed' exponential relaxation has been reported for a variety of glassy or jammed systems, ranging from attractive colloidal gels and packed repulsive soft spheres to polymer or molecular glass formers (for reviews, see e.g. [2, 3]). These dynamics are typically supradiffusive or even ballistic and their origin has been often ascribed to internal stress relaxation, although little direct evidence has been provided for the progressive relaxation or even the very existence of internal stress in these materials.

In this talk, I'll first describe the new experiments by Ruta *et al.* [1] and then review past work on glassy ballistic dynamics. Finally, I'll discuss recent measurements [4] of the dynamics and rheological properties of actin networks, which exhibit compressed exponential relaxation. Using a combination of optical microscopy and non-conventional space-resolved light scattering, we show that in actin networks the slow evolution of mechanical properties is accompanied by the relaxation of strain field and ballistic microscopic dynamics. Our experiments provide evidence of the existence and the progressive relaxation of internal stress in a material exhibiting anomalous supradiffusive dynamics, thereby lending support to the notion that stress relaxation is a key ingredient in structural relaxation of glassy and jammed systems.

This work is the result of very fruitful and stimulating collaborations with many students, postdocs, and colleagues. I'm in particularly deeply indebt to B. Ruta, G. Monaco, G. Brambilla, O. Lieleg, J. Kaiser, and A. Bausch. Funding from ANR and CNES is gratefully acknowledged.

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[2] L. Cipelletti and L. Ramos, J. Phys. : Condens. Matter **17**, R253 (2005).
[3] A. Madsen *et al.*, New J. Phys. **12**, 055001 (2010).
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Friday

09:00 – 10:30 Anomalous Transport

Chair: Thomas Voigtmann

J1	**Ralf Metzler**	*Ageing and ergodicity breaking in anomalous diffusion*
J2	**Felix Höfling**	*Anomalous transport, localisation, and long-time tails in heterogeneous media*
J3	**Georg Maret**	*Anomalous transport and Anderson localization of light in strongly scattering media*

10:30 – 11:00 Coffee break

11:00 – 12:30 Granular Matter II

Chair: Thomas Franosch

K1	**Hans Herrmann**	*Understanding aeolian saltation through simulations*
K2	**Jean-Louis Barrat**	*Viscosity divergence and jamming transition in athermal suspensions*
K3	**Matthias Sperl**	*Dynamics of Granular Matter under Homogeneous Agitation*

12:30 – 12:45 Closing Remarks

J1 **Ralf Metzler** **09^{00} – 09^{30}**

Ageing and ergodicity breaking in anomalous diffusion

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In 1905 Einstein formulated the laws of diffusion, and in 1908 Perrin published his Nobel-prize winning studies determining Avogadro's number from diffusion measurements. With similar, more refined techniques the diffusion behaviour in complex systems such as the motion of tracer particles in living biological cells or the tracking of animals and humans is nowadays measured with high precision. Often the diffusion turns out to deviate from Einstein's laws [1]. This talk will discuss the basic mechanisms leading to such anomalous diffusion as well as point out its consequences. In particular the unconventional behaviour of non-ergodic, ageing systems will be discussed within the framework of continuous time random walks [2, 3]. Indeed, non-ergodic diffusion in the cytoplasm of living cells as well as in membranes has recently been demonstrated experimentally [4]. There also exist ergodic anomalous diffusion processes, such as fractional Brownian motion or diffusion on a fractal. These represent physically different mechanisms. The behaviour of time averages of such processes will be discussed [5], and methods to distinguish different processes presented [6].

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J2 **Felix Höfling** **$09^{30} - 10^{00}$**

Anomalous transport, localisation, and long-time tails in heterogeneous media

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Aubiquitous observation in biological cells is that the diffusive motion of macromolecules and organelles is anomalous, and a description simply based on the conventional diffusion equation with diffusion constants measured in dilute solution fails [1]. This is commonly attributed to “macromolecular crowding” in the interior of cells and in cellular membranes, summarising their densely packed and heterogeneous structures. The most familiar phenomenon is a sublinear, power-law increase of the mean-square displacement as function of the lag time, but there are other manifestations like strongly reduced and time-dependent diffusion coefficients, persistent correlations in time, non-gaussian distributions of spatial displacements, heterogeneous diffusion, and the presence of immobile particles. There is a large body of recent experimental evidence for anomalous transport in crowded biological media: in cyto- and nucleoplasms as well as in cellular membranes, complemented by *in vitro* experiments where a variety of model systems mimic physiological crowding conditions. Similarly, transport in spatially heterogeneous materials such as rocks, soils, gels, and ceramics is strongly hindered and often anomalously slow.

A microscopic picture underlying the phenomenologically observed anomalous transport is yet to be established. One possible origin is the highly obstructed motion in the ramified, heterogeneous environment, the essence of which is captured by the Lorentz model. There, tracer particles move in a spatially heterogeneous medium which is idealised by randomly distributed obstacles (Fig. 1). Slow dynamics and anomalous transport emerge generically over the full range of packing fractions [2]. The model exhibits a localisation transition where the tracer transport ceases upon approaching a critical packing fraction. The transition induces subdiffusive motion, which is observed over many decades in time close to the critical point. The dynamics is rationalised in terms of a cluster-resolved scaling theory [3] and is characterised by a set of universal exponents. Further, the non-ergodicity parameter displays a singularity at the transition; the tracer motion is, however, non-ergodic at *all* packing fractions due to particles being trapped in closed pockets.

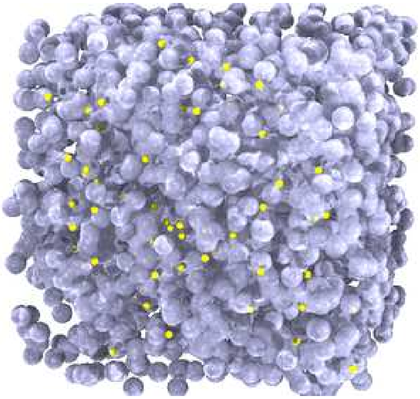

FIG. 1. Tracer particles exploring a heterogeneous medium made of randomly distributed, overlapping spheres.

The velocity autocorrelation function (VACF) $Z(t)$ is characterised by the competition of a critical power law, associated with the subdiffusive motion, and a universal long-time tail, $-Z(t) \sim t^{-d/2-1}$ [4]. For the latter, rigorous results exist in the dilute limit for scattering off frozen obstacles and similarly for an overdamped colloidal suspension. These calculations can be interpreted such that the tail emerges from repeated encounters with the same scatterer. Harnessing the compute power of high-end graphics processors [5], we have numerically investigated the dynamics of a tagged particle in the binary Kob–Andersen mixture upon cooling. As the glass transition is approached, our data corroborate the emergence of a power-law decay of the VACF with exponent 5/2 and negative prefactor—reminiscent of the tail in the Lorentz model [6]. The power law is well developed in a VACF restricted to the most *immobile* particles, while the most *mobile* ones essentially do not contribute, but display persistent positive correlations instead. We speculate that the Lorentz-like power law decay is closely related to

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the cage effect and infer the coexistence of quasi-arrested cages and fluid-like regions.

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J3 **Georg Maret** **$10^{00} - 10^{30}$**

Anomalous transport and Anderson localization of light in strongly scattering media

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In the diffusive transport of waves in three dimensional disordered media a phase transition with increasing disorder from a conducting to a non conducting (localized) state was predicted by P.W. Anderson in 1958 [1] in the context of electronic transport [1]. Later, it was realized that this type of localization should be generic for all types of waves including light [2, 3]. The quest for the experimental demonstration of Anderson localization of waves in 3D media has been a challenging task ever since. For electrons [4] and cold atoms [5] the difficulty lies in the competing possibility of bound states in valleys of the disordered potential. Classical waves such as electromagnetic and acoustic waves have thus been prime candidates for the observation of Anderson localization in 3D [6–10], but the main challenge is to distinguish between effects of absorption and localization [9, 10]. Time resolved transmission measurements provide such a distinction, in principle, since localization delays the typical transit times of a brief incident photon pulse while absorption shortens them [11, 12].

Here we present measurements of the time- dependence of the transverse width of the waves transmitted through strongly turbid slabs, which provides a direct measure of the localization length and is independent of absorption. From this we find direct evidence for a localization transition in three dimensions and determine the corresponding localization lengths. In the diffusive regime ($kl^* \gg 1$) the mean square width σ^2 of the transmitted pulse, i.e. the spread of the photon cloud, follows the expected linear increase in time $\sigma^2 = 4Dt$. Here, D is the diffusion coefficient for light, k the wave-vector and l^* the transport mean free path. With increasing turbidity $1/kl^*$ the width σ^2 increases subdiffusively at long times and finally saturates towards a plateau value identified by the localization length ξ. From the $1/kl^*$-dependence of this behavior we determine the transition to occur at $kl^* \approx 4.5$ for our system, in good accord with earlier work [12, 13] and determine the critical exponent of the transition to be close to unity. When the thickness L of the sample becomes comparable to ξ a decrease of the width of the photon distribution is observed at long times. This surprising fact can be qualitatively understood in a statistical picture of localization, where a range of localization lengths exists in the sample corresponding to different sizes of closed loops of photon transport. In finite thickness slabs larger localized loops will be cut off by the surfaces leading to a lower population of such localized states at longer times. Therefore, such data yield valuable information about the statistical distribution of localization lengths close to the transition.

We acknowledge fruitful discussions with Nicolas Cherroret and financial support by DFG, SNSF and the Center for Applied Photonics (CAP).

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K1 **Hans J. Herrmann** **$11^{00} – 11^{30}$**

Understanding aeolian saltation through simulations

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We study numerically aeolian saltation which is the transport mechanism of sand dunes. The mesoscopic approach via DEM not only provides a novel and precise insight of the particle splash, but also strikingly unveils that mid-air collisions between saltation grains enhance the particle flux. A spherical particle bed of disordered layers is dragged by a logarithmic velocity field that mimics the wind profile. The integral of the forces $\mathbf{F}_d$ applied to every particle in the x-direction gives the grain stress $\tau_g(y)$ for a certain height y.

$$\tau_g(y) = \sum_{y}^{\infty} \frac{\mathbf{F}_i}{A}, \quad \text{with} \quad \mathbf{F}_i = -\frac{\pi D_i^2}{8} \rho_a C_d v_r \mathbf{v_r}, \tag{1}$$

where A is the cross-sectional area parallel to the ground, ρ_a the air density, C_d the drag coefficient, and $\mathbf{v_r} = \mathbf{v} - \mathbf{u}$ the velocity difference between particle and wind, with $v_r = |\mathbf{v_r}|$. The modified wind shear velocity $u_\tau(y)$ corresponds to the fluid stress left at the height y after the momentum transfer between wind and particles,

$$u_\tau(y) = u_* \sqrt{1 - \frac{\tau_g}{\rho_a u_*^2}}. \tag{2}$$

The modified shear velocity provides the differential form of the modified wind profile,

$$\frac{du}{dy} = \frac{u_\tau(y)}{\kappa y}, \tag{3}$$

where $\kappa = 0.4$ the von Kármán constant.

A detailed study on the splash shows that fast particles, called saltons (yellow particle in Fig. 1) hop over a granular packing initially at rest and eject several other particles. The kinetic energy of the saltons must be able eject other particles despite the substantial dissipation in the particle bed. The leapers are lifted and accelerated by the wind making some small jumps (red particles), the creepers solely roll over the surface of the bed (green particles). For low wind shear velocities, saltons may not have the kinetic energy necessary to eject others, and suspend the saltation. Such interruption may also depend on the packing configuration of the particles. The combination of these two factors explains why the transition on the impact threshold of the saturated flux, previously assumed to be continuous, is found to be in fact discontinuous [1].

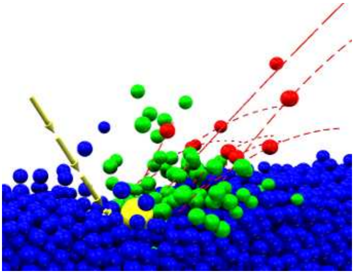

FIG. 1. Typical splash obtained numerically in 3D.

After successive impacts of the salton with the ground, a cloud of leapers raises. The leapers collides with each other due to the decrease of the mean free path and the first saltons appear. The collisions between leapers shoot saltons over the cloud, which sustains the motion of the saltons. The flux increase comes from the stronger acceleration from the wind to the saltons at the higher positions. An example of the two trajectories is shown in Fig 2. Creapers and leapers also contribute both considerably to the global sand flux. Futhermore, we verified a bimodal and continuous splash distribution with a broad spectrum of slow particles and a small peak of fast ones as also observed by Anderson and Haff previously.

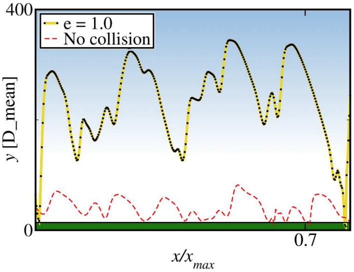

FIG. 2. Particle trajectories in a model with elastic mid-air collisions ($e = 1$) and without mid-air collisions (red).

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K2 **Jean-Louis Barrat** **$11^{30} - 12^{00}$**

Viscosity divergence and jamming transition in athermal suspensions

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Many materials, from emulsions and suspensions to foams and granular materials are dense assemblies of non-Brownian particles. Since thermal energy is irrelevant, the dynamics of these systems must be studied in driven non-equilibrium conditions. Together with the driving mechanism, a second important control parameter is the volume fraction of the particles, ϕ. These materials undergo a fluid-to-solid 'jamming' transition as ϕ increases beyond some critical density ϕ_c.

In order to investigate the universal aspects of this transition, the behavior of a simple model for non Brownian suspensions of hard disks in shear flow has been studied using extensive numerical simulations, both quasistatic and at finite strain rates. A continuous jamming transition from a freely flowing state to a yield-stress situation takes place at a well-defined packing fraction, where the scaling characteristic of isostatic solids is observed [1]. The particle motion becomes strongly heterogeneous at the transition, with a characteristic length scale that diverges algebraically. Single particle displacement display an interesting crossover from ballistic to diffusive, which involves a similar length scale [2].

An important property of the jamming transition is the algebraic divergence in the viscosity that takes place at ϕ_c [3]. It is proposed that this divergence is dominated by fluctuations in the particle velocities, that control the dissipation rate. These fluctuations are similar in quasi-static simulations and for finite strain rate calculations with various damping schemes. Hence the statistical properties of grain trajectories – in particular the critical exponent of velocity fluctuations with respect to volume fraction ϕ – are determined by steric effects, which are the only ingredient in the quasistatic simulations. Again, the divergence can be related to a diverging length scale, and the exponent obtained from simulations of our simple model is in good agreement with the one observed in experiments [4].

This work is the outcome of collaborations with Dr Claus Heussinger (Göttingen), Dr Ludovic Berthier (Montpellier) and Prof. Bruno Andreotti (Paris). Support from Institut Universitaire de France and from the Feodor Lynen program of the von Humboldt foundation are acknowledged.

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K3 **Matthias Sperl** **$12^{00} - 12^{30}$**

Dynamics of Granular Matter under Homogeneous Agitation

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Granular particles loose energy during their collisions among each other and with the walls of the container. This energy loss needs to be compensated by energy input from external driving to prepare well-defined initial or steady states. Similar to the development of classical fluid dynamics, theoretical descriptions for granular matter started with dilute systems known as granular gases. Both theoretical and numerical work have predicted a great number of novel phenomena for such granular gases [1]. However, even some of the most essential predictions have remained untested, since well-defined experimental environments are missing in ground-based experiments. While under gravity, granular particles sediment quickly and cannot be agitated without large gradients (cf. Fig. 1 left), in microgravity, homogeneous agitation is possible, cf. Fig. 1 right.

In the experiment MEGraMa (Magnetically Excited Granular Matter), granular particles are excited by magnets surrounding a cubic test cell. The magnetic excitation is used to prepare well-defined experimental conditions, and the particle dynamics is investigated by highspeed imaging either in the steadily driven state or after magnetic driving is switched off. It is demonstrated that magnetic excitation can prepare homogeneous granular states reliably.

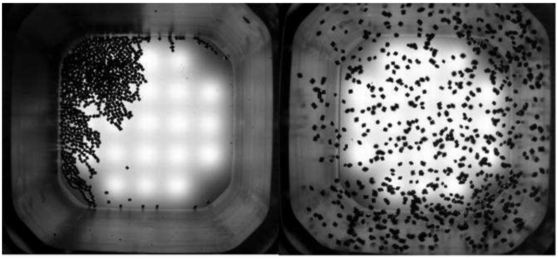

FIG. 1. Agitated granular particles on a parabolic flight under 1g (left) and 0g (right).

Using magnetic excitation to prepare homogeneous granular gases under microgravity (on parabolic flight and drop tower), the following phenomena are observed: (1) the velocity distribution in granular gases is smooth but deviates from the Maxwell distribution both in steady states and during cooling, (2) the celebrated Haff cooling law, cf. Eq. (1) is demonstrated experimentally, and (3) granular gases of strongly aspherical particles display arrested dynamics even in the very dilute limit.

The cooling law for a granular gas according to Haff [2] describes the decrease of the average velocity $\bar{v}(t)$ with time t in a homogeneously cooling granular gas as

$$\bar{v}(t) = \frac{v_0}{1 + t/\tau_{\text{Haff}}} \tag{1}$$

where v_0 is the initial average velocity and τ_{Haff} is the characteristic time scale that depends on microscopic parameters.

We thank the space agencies DLR and ESA for continued support and flight opportunities.

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