DY 56: Poster: Glasses; Granular Matter; Brownian Motion and Anomalous Diffusion

Time: Thursday 15:00–18:00 Location: P1A

DY 56.1 Thu 15:00 P1A

Stationary current in the open Bose-Hubbard chain — Anna Bychek[1], Pavel Muraev[2], Dmitrii Maksimov[1,3], and •Andrey Kolovsky[1,2] — [1]Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia — [2]Siberian Federal University, 660041 Krasnoyarsk, Russia — [3]Siberian State Aerospace University, 660014 Krasnoyarsk, Russia

We analyze stationary current of bosonic carriers in the Bose-Hubbard chain of length L where the first and the last sites of the chain are attached to reservoirs of Bose particles acting as the particle source and sink, respectively. The analysis is curried out by using the pseudoclassical approach which reduces the original quantum problem to the classical problem for L coupled nonlinear oscillators. It is shown that an increase of oscillator nonlinearity (which is determined by the strength of inter-particle interactions) results in a transition from the ballistic transport regime, where the stationary current is independent of the chain length, to the diffusive regime, where the current is inverse proportional to L.

DY 56.2 Thu 15:00 P1A

Analytical theory for predicting variations of activation energies in mixed glass former glasses — •Julian Fischer, Marco Bosi, and Philipp Maass — Fachbereich Physik, Universität Osnabrück, Germany

The mixed glass former effect manifests itself in a nonadditive behaviour of physical and chemical properties upon mixing of two or more different glass formers in ion-conducting glasses[1]. Most striking is the behaviour of conductivity activation energies. They can exhibit minima at certain mixing ratios that at room temperature lead to enhancements of ionic conductivities by several orders of magnitude compared to the respective glasses containing only one of the network formers.
We present an analytical approach for modeling the variation of conductivity activation energies $E_a(x)$ with the glass former mixing ratio x. This approach is based on the assumption that changes of the free energy landscape for the long-range ion transport are governed by changes of the concentration of glass former units[2]. Theoretical results obtained by adjustment of only one parameter are in surprisingly good agreement with experimental findings.

[1] M.D. Ingram, Phys. Chem. Glasses 28, 215 (1987).
[2] M. Schuch, C. Trott, P. Maass, RSC Adv. 1, 1370 (2011).

DY 56.3 Thu 15:00 P1A

Collective single-file transport in periodic potentials — •Dominik Lips[1], Artem Ryabov[2,3], and Philipp Maass[1] — [1]Universität Osnabrück, Germany — [2]Charles University, Prague, Czech Republic — [3]Universidade de Lisboa, Portugal

Driven lattice gases are often used to model single-file molecular transport and biological traffic. With respect to continuous space dynamics, the discrete lattice can be regarded to represent a periodic energy landscape in a coarse-grained manner. Thermally activated transitions of particles between different potential wells correspond to jumps between lattice sites, while effects on length scales smaller than the lattice constant are neglected. To study single-file transport on a lower level of coarse-graining, the Brownian asymmetric simple exclusion process (BASEP) was recently introduced [1,2]. In this BASEP, hard spheres perform a driven Brownian motion in a periodic potential under a constant drag force. Case studies with a cosine potential show that the collective dynamics depend sensitively on the ratio of the particle size and wave length of the potential. The interplay of three physical mechanisms leads to a rich variety of nonequilibrium phase transitions in open systems [1,2], and counterintuitive short uphill transitions [3]. Here, we report on new results obtained for periodic potentials with multiple minima per period and other short-range interactions.
[1] D. Lips, A. Ryabov, P. Maass, Phys. Rev. Lett. **121**, 160601 (2018).
[2] D. Lips, A. Ryabov, P. Maass, Phys. Rev. E **100**, 052121 (2019).
[3] A. Ryabov, D. Lips, P. Maass, J. Phys. Chem. C **123**, 5714 (2019).

DY 56.4 Thu 15:00 P1A

The role of initial speed in projectile impacts into light granular media — •Kai Huang[1,2], Dariel Hernadez Delfin[3], Felix Rech[1], Valentin Dichtl[1], and Raul Cruz Hidalgo[3] — [1]Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany — [2]Division of Natural and Applied Sciences, Duke Kunshan University, 215306 Kunshan, Jiangsu, China — [3]Department of Physics and Applied Mathematics, University of Navarra, 31009 Pamplona, Spain

Projectile impact into a light granular material composed of expanded polypropylene (EPP) particles is investigated systematically with various impact velocities. Experimentally, the trajectory of an intruder moving inside the granular material is monitored with a recently developed microwave radar system noninvasively. Numerically, discrete element simulations together with coarse-graining techniques are employed to address both dynamics of the intruder and response of the granular bed. Our experimental and numerical results of the intruder dynamics agree with each other quantitatively and are in congruent with existing phenomenological model on granular drag. Stepping further, we explore the 'microscopic' origin of granular drag through characterizing the response of granular bed, including density, velocity and kinetic stress fields at the mean-field level. The macroscopic profiles of the granular bed ahead of the intruder decays exponentially in the co-moving system of the intruder, giving rise to a characteristic length scale on the order of intruder size.

DY 56.5 Thu 15:00 P1A

Interpreting impedance spectroscopy data by using Poisson-Nernst-Planck anomalous models — Ervin K. Lenzi[1], Luiz R. Evangelista[2], Leila Taghizadeh[3], Daniel Pasterk[3], Rafael S. Zola[4], Trifce Sandev[5,6,7], Clemens Heitzinger[3], and •Irina Petreska[7] — [1]Universidade Estadual de Ponta Grossa — [2]Universidade Estadual de Maringá — [3]Technische Universität Wien — [4]Universidade Tecnológica Federal do Paraná — [5]Macedonian Academy of Sciences and Arts — [6]University of Potsdam — [7]Ss. Cyril and Methodius University in Skopje

The information obtained from impedance spectroscopy of electrolytic cells enables comprehension of the complex diffusion phenomena in liquid/solid interfaces. In this context, we consider two implementations of the Poisson-Nernst-Planck (PNP) anomalous models of the electrical response of electrolytic cells, one built in the frameworks of the fractional calculus and the other one being an extension of the standard PNP model presented by Barsoukov and Macdonald. Both extensions may be related to an anomalous diffusion with subdiffusive characteristics through the electrical conductivity and are able to describe the experimental data. Bayesian inversion is also applied to extract the parameter of interest in the analytical formulas of impedance, using the delayed-rejection adaptive-Metropolis algorithm (DRAM) in the context of Markov-chain Monte Carlo (MCMC) algorithms to find the posterior distributions and confidence intervals.
[1] E. K. Lenzi et al., J. Phys. Chem. B 123, 7885 (2019).

DY 56.6 Thu 15:00 P1A

Diffusion in combs with stochastic resetting — •Viktor Domazetoski[1], Axel Masó-Puigdellosas[2], Trifce Sandev[1,3,4], Vicenç Méndez[2], Alexander Iomin[5], and Ljupco Kocarev[1,4] — [1]Macedonian Academy of Sciences and Arts — [2]Universitat Autónoma de Barcelona — [3]University of Potsdam — [4]Ss. Cyril and Methodius University in Skopje — [5]Technion, Haifa

Diffusion on a three dimensional xyz–comb is analyzed. Three different types of resetting are considered. These are: (i) global resetting to the initial position, (ii) resetting to the x–backbone, and (iii) resetting to the main y–fingers. Analyzing the probability density functions, their stationary distributions and the mean squared displacements, we observe different transient dynamics along the backbone in all three cases of the resetting mechanisms. The main conclusions from the analysis are as follows. The global resetting breaks the transport in all three directions, while the resetting to the backbone breaks the transport in two (y and z) directions but enhances the transport in the main x–axis. Moreover, the resetting to the z–fingers enhances the transport in the backbone and the main y–fingers, while the transport along the z–fingers is localized, when the mean squared displacement reaches a steady value. The analytical results are confirmed by numerical simulations in the framework of coupled Langevin equations for the comb structure.

DY 56.7 Thu 15:00 P1A

Unknotting of quasi-two-dimensional ferrogranular networks by in-plane homogeneous magnetic fields — Pedro A. Sanchez[1,2], Justus Miller[3], Sofia S. Kantorovich[4], and •Reinhard Richter[3] — [1]Ural Federal Univ., 51 Lenin av., Ekaterinburg, 620000, Russian Federation — [2]Inst. of Ion Beam Physics and Materials Research, H-Z Dresden-Rossendorf e.V., 01314 Dresden, Germany — [3]Experimentalphysik 5, Univ. of Bayreuth, 95440 Bayreuth, Germany — [4]Computational Physics, Univ. of Vienna, 1090 Vienna, Austria

We are exploring in experiments and computer simulations, the aggregation process in a shaken granular mixture of glass and magnetized steel beads, occuring after the shaking amplitude is suddenly decreased. Then the magnetized beads form a transient network that coarsens in time into compact clusters, following a viscoelastic phase separation [1]. Here we focus on the quasi-two-dimensional case, analyzing in computer simulation the effects of a magnetic field parallel to the system plane [2]. Our results evidence that the field drastically changes the structure of the forming network: chains and elongated clusters parallel to the field are favored whereas perpendicular connecting structures tend to be supressed, leading to the unknotting of the networks familiar from zero fields. By means of a field dependent orientation parameter we compare numerical and experimental results.

[1] A. Kögel, et al. *Soft Matter*, 14 (2018) 1001.

[2] P. A. Sánchez, J. Miller, S. S. Kantorovich, R. Richter, *J. Magn. Magn. Mater*, accepted (2019).

DY 56.8 Thu 15:00 P1A

System size scaling of a model glass under shear — •Moumita Maiti[1], Lawrence Smith[2], and Andreas Heuer[3] — [1]Institute of Physical Chemistry, UNiversity of Muenster, Muenster,Germany — [2]Institute of Physical Chemistry, UNiversity of Muenster, Muenster, Germany — [3]Institute of Physical Chemistry, UNiversity of Muenster, Muenster, Germany

We simulate a binary Lennard-Jones glass under shear for different system sizes with a very low shear rate at a temperature close to zero. We observe shear bands for larger system sizes. The tails of the Van-Hove function of such samples display a scaling with the system size with an exponent 0.5. We relate the scaling to the presence of activating shear transformation zones (STZs) and speculate about the impact of the coupling of different STZs as the source of these finite size effects. This is further corrobated by analyzing the number of fast moving particles. We anticipate a positive correlation between the number of activated STZs and the number of single particle jumps. We observe that the number of jumps per particle scales with system sizes too but with a different exponent 0.25. We discuss possible reasons for the difference of the two scaling exponents.

DY 56.9 Thu 15:00 P1A

Accurate determination of local properties in 2D particulate systems using Set Voronoi tessellation — •Simeon Völkel[1] and Kai Huang[1,2] — [1]Universität Bayreuth, Experimentalphysik V, Universitätsstraße 30, 95447 Bayreuth, Germany — [2]Duke Kunshan University, Division of Natural and Applied Sciences, No. 8 Duke Avenue, Kunshan, Jiangsu, China 215316

Using the collective behavior of a granular rod monolayer under vertical vibrations, we demonstrate the advantages of the Set Voronoi tessellation in two dimensions (2D).

The behavior of particulate systems typically depends critically on the *local* configuration of its constituents, requiring accurate measurements of properties such as bond orientational order parameters or the local volume fraction. In this regard, Voronoi tessellation is a common tool for tiling space, but is only appropriate for mono-disperse spheres. This severely limits its applicability, especially in dense systems of poly-disperse and non-spherical particles, which are commonly found in practice. To overcome this limitation, Set Voronoi was proposed which assigns points in space according to the closest particle surface (contour for the 2D case) instead of closest particle center.

We show that Set Voronoi delivers consistent results even for extreme cases, where the error in the local volume fraction obtained using classical Voronoi goes up to 100 %. Our 2D implementation can be applied directly to a variety of (quasi-)2D particulate systems of practical interest ranging from granulates to pedestrian and traffic flow systems.

DY 56.10 Thu 15:00 P1A

Superdiffusion in Kac-Zwanzig heat baths — •Paul Ledwon and Igor Sokolov — Institut für Physik, Humboldt Universität zu Berlin

We consider the Kac-Zwanzig heat bath model, an ensemble of harmonic oscillators interacting with a single distinguished particle. The model is known to allow for rigorous derivation of the generalized Langevin equation (GLE) from the underlying Hamilton dynamics in the thermodynamic limit. The memory kernel of this equation depends on the distribution of the spring constants and masses of the bath oscillators, and on their interaction strengths with the distinguished particle. Our specific focus is on the memory kernels leading to superdiffusion of the distinguished particle, in which mean squared displacement grows faster than linearly in time. We discuss restrictions on the parameters on the bath including its size necessary for effectively simulating superdiffusion, and the algorithmic implementation of the corresponding simulations.

DY 56.11 Thu 15:00 P1A

Angle of repose of granular materials: Analytical expression from Molecular Dynamic simulations — Filip Elekes and •Eric Josef Ribeiro Parteli — Department of Geosciences, University of Cologne

The angle of repose is one of the most important quantities used to characterize the packing behavior and flowability of granular materials in industrial applications, environmental sciences and planetary research. However, the dependence of this angle on particle size and gravity remains poorly understood. Here we investigate the angle of repose of granular materials by means of particle-based simulations. Our model includes contact forces as well as non-bonded attractive inter-particle forces due to van der Waals interactions. From our simulations, we obtain a mathematical expression that predicts the angle of repose θ_r of spherical particles as a function of particle size and gravity. We find excellent agreement between predicted and experimentally observed values of θ_r for the investigated values of particle diameter within the broad range between 30 μm and 1 cm. Moreover, our results shed new light into experimental observations of the angle of repose on Mars and other extra-terrestrial environments.

DY 56.12 Thu 15:00 P1A

Coexistence of fixed and active dunes from numerical simulations — Maria Determann and •Eric Josef Ribeiro Parteli — Department of Geosciences, University of Cologne

The side-by-side coexistence of fixed and active Aeolian dunes in many environmental settings of the Earth defies our understanding of dune mobility as proxy for regional climate and environmental conditions. According to this understanding, fixed dunes prevail if the characteristic vegetation cover growth rate in a given region exceeds twice the rate of surface erosion and deposition processes caused by Aeolian transport, while dunes are predicted active otherwise. Here we show, by means of numerical simulations, that coexistence between stabilized and active dunes can be explained by climate-driven oscillations in atmospheric forcing relative to stabilizing vegetation growth conditions. The underlying factor for this co-existence is the hysteresis in the stabilization process of Aeolian dunes, i.e., much stronger winds are needed to reactivate fixed dunes than the ones required to stabilize them. Our simulations reproduce regional patterns of coexisting fixed and active dunes occurring under seasonal oscillation of rainfall and wind power, without requirement of any assumption on spatial heterogeneities in soil fertitility.

DY 56.13 Thu 15:00 P1A

Athermal Jamming for particles with exponentially decreasing repulsions — •Nicolas Wohlleben and Michael Schmiedeberg — Institut für Theoretische Physik I, FAU Erlangen-Nürnberg, Germany

We study the jamming of a colloidal system where the particles interact according to a Yukawa potential, i.e., the repulsion decreases exponentially with the distance as expected for screened Coulomb interactions of charged colloids in solution. The decay occurs on a length scale given by the screening length and in addition we consider a cutoff length where the potential is set to zero in a smooth way as often used in simulation.

By determining the athermal jamming transition by trying to remove overlaps we find that the transition packing fraction only depends on the cutoff length but hardly on the screening length. We also explore the radial distribution function and again confirm the importance of the cutoff length.

The picture that emerges is that the influence of a cutoff length on

athermal jamming is superior to that of the screening length, although the screening length is expected to control the slowdown of the dynamics (i.e., the dynamical glass transition). As a consequence, athermal jamming (as defined by overlaps) and the glass transition obviously are unrelated in the considered system.

DY 56.14 Thu 15:00 P1A

Polybutadiene confined in alumina pore — •Lama Tannoury and Wolfgang Paul — Martin Luther Universität

Several studies concerning 1,4-polyutadiene (PBD) confined between graphite walls have been performed perviously. They have shown that the polymer melts experience, at close distances to the confining walls, a variation in both monomer and chain density. Furthermore, that layer also experiences a change in dynamics incorporated in the slowing down of and an extra process of relaxation. These studies are essential to the comprehension of composite materials made of polymer matrices and inorganic filler particles such as rubber tires. The latter is a composite material filled with nanoparticles. However, since previous research on PBD melts permeated by nano-sized fillers could not reach relaxation time scales accessible by MD simulations, we attempt to study a chemically realistic model of a PBD melt inside alumina and silica pores using the GROMACS package. We aim to enhance our view concerning bulk relaxation processes and any modifications they experience due to confinement.