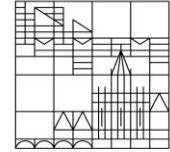# Kolloquium

Theoretische Physik
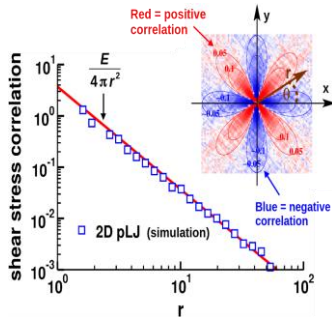
Universität
Konstanz

Prof. Dr. Jörg Baschnagel
Institut Charles Sadron (France)

Mo 29.01.24
13:30 Uhr
P 603

Correlations of stress fluctuations in glass-forming liquids.

Many fluids do not crystallize upon cooling, but form amorphous, glassy, solids at low temperature. As liquids, amorphous solids are on average isotropic so that static pair-correlation functions do not allow to distinguish between fluid and solid states. However, a distinction is possible under weak shear deformation which make a fluid flow, while a solid deforms elastically. Glass-forming liquids "interpolate" between fluid and solid behavior, as the slowing down of the dynamics on cooling is accompanied by the emergence of elastic features. To characterize this viscoelasticity the spatio-temporal correlation function $C_{xyxy}(r,t)$ of the local shear stress, for vectorial distance r and time t, has attracted a lot of recent interest. The talk is embedded in this topical context. We examine a two-dimensional (2D) polydisperse Lennard-Jones (pLJ) model for a glass-forming system. The model is studied by molecular simulations (molecular dynamics and Monte Carlo) [1,2] and theory [2,3]. Our major results are: At low temperature and long times, $C_{xyxy}(r,t)$ does not depend on $r = |r|$ only, but also on the angle θ of the vector r with the x axis (cf. inset in the figure). In agreement with other recent work [Lemaître, JCP (2018); Maier, Fuchs, Zippelius, JCP (2018)], we argue that this behavior arises because the system is isotropic and achiral. The octupolar dependence of $C_{xyxy}(r,\theta)$ on the angle θ, visible by the sequence of negative (blue) and positive (red) correlations in the inset of the figure above, is thus a necessary consequence for isotropic and achiral systems. (ii) Specifically chosen angular averages allow to extract the dependence of $C_{xyxy}(r,\theta)$ on r. This dependence is long-ranged, decaying as $1/r^2$ in 2D with an amplitude being given by a particular elastic constant, the Young modulus E. Our theory (lines) is in good agreement with the simulation results (main figure: symbols; inset: pixels) [3].

Host: Prof. Matthias Fuchs

•J. P. Wittmer, A. N. Semenov, J. Baschnagel, Phys. Rev. E **108**, 015002 (2023).

•L. Klochko, J. Baschnagel, J. P. Wittmer, H. Meyer, O. Benzerara, A. N. Semenov, J. Chem. Phys. **156**, 164505 (2022).

•L. Klochko, J. Baschnagel, J. P. Wittmer, A. N. Semenov, Soft Matter **14**, 6835 (2018).