Long-range stress and strain correlations in simulated polymer melts and networks

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Research context: The theory and simulation group at the Institut Charles Sadron (ICS) is quite generally interested in the statistical physics and rheology of soft matter and complex fluids with a particular emphasis on long-range static and dynamical correlations in polymer solutions and melts [1]. Using simple coarse-grained models many fundamental and generic aspects can be investigated by means of molecular dynamics or Monte Carlo simulations.

Scientific background: The characterization of disordered materials boils down to the measurement and prediction of correlation functions of tensorial fields characterizing, e.g., second-order stress and strain fields [3,4]. Importantly, correlation functions of tensor fields for isotropic systems transform differently under orthogonal transformations than correlation functions of scalar fields. It is thus crucial to characterize in a first step the "Invariant Correlation Functions" (ICFs) to avoid any spurious dependence on the coordinate system [2-4]. The ICFs for stress and strain fields in polymer melts and networks can be traced back analytically in the hydrodynamic limit to two rheological material functions [2]. This leads (under rather general conditions) to long-range stress and strain correlations decaying as $1/r^d$ (r=distance between two field points, d=spatial dimension). These universal viscoelastic correlations have already been shown crucial for the short-chain melt dynamics [1].

Proposed PhD: The aim of the proposed PhD study is to characterize numerically in reciprocal space the ICFs of the stress and strain fields of dense polymeric systems

- starting first with the polymer networks permanently cross-linked by ideal springs,
- moving then to systems with reversible (transient) cross-links
- and finally to long polymer melts (entangled merely due to topological constraints).

It is also important to characterize the time-dependence of the ICFs. The proposed numerical methodology, never been used so far for polymer systems, is also relevant for isotropic non-equilibrium driven systems where statistical mechanics has to be used with care.

In a nutshell: We are seeking to fill a PhD position for mainly numerical work on long-ranged strain and stress correlations in simulated polymer melts and networks aiming to test and to refine recent theoretical predictions.

[1] J. Farago, H. Meyer, A.N. Semenov, *Anomalous diffusion of a Polymer Chain in an Unentangled Melt*, Phys. Rev. Lett., **107**, 178301 (2011).

[2] L. Klochko, J. Baschnagel, J.P. Wittmer, A.N. Semenov, *Long-range stress correlations in viscoelastic and glass-forming fluids*, Soft Matter, **14**, 6835 (2018).

[3] J.P. Wittmer, J. Baschnagel, A.N. Semenov, *Correlations of tensor field components in isotropic systems with an application to stress correlations in elasti bodies*, Phys. Rev. E, submitted (2023).

[4] J.P. Wittmer, J. Baschnagel, A.N. Semenov, *Strain correlations in isotropic elastic bodies*, Soft Matter, submitted (2023).