Stress correlations in glass-forming liquids

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Background. Many liquids cooled to low temperature do not crystallize, but stay amorphous upon freezing. The amorphous solid is called “glass”. On cooling the liquid toward the glass, the viscosity of the liquid increases dramatically. Since the viscosity can be expressed as the time-integral over the shear relaxation modulus $G(t)$, the increase of the viscosity implies that the decay of $G(t)$ with time t strongly slows down. Recent studies [1–3] reveal that this slowing down is related to the emergence of elastic features, typical of solids, in the cold liquid. The studies also suggest that these solid-like features are accompanied by long-range spatial correlations that can be probed by the wave-vector ($\boldsymbol{q}$) and time dependent correlation function $\boldsymbol{C}(\boldsymbol{q},t)$ of the shear stress. This function is tensorial in nature and encapsulates the intricate interplay of relaxation phenomena (via t) and structural correlations (via $\boldsymbol{q}$) of the local shear stress. It is an appealing candidate to unravel hidden spatio-temporal correlations underlying the transition from the liquid to the glass, a topical problem in current condensed matter physics [4].

PhD project. The project builds on ongoing work in our group [3,7]: It will employ Monte Carlo (swap algorithm [5]) and molecular dynamics simulations of two-dimensional (2D) polydisperse Lennard-Jones (LJ) systems to explore the spatio-temporal correlations of the shear stress. The effects of the equilibration procedure (slow cooling vs. swap) will be analysed in detail. Since the correlations are expected to be of long range, several large systems have to be studied, up to the largest sizes currently feasible [6]. An efficient implementation of $\boldsymbol{C}(\boldsymbol{q},t)$ and its finite-size analysis need to be carried out. While 2D systems allow for large sizes, they feature long-range correlations, first recognized by Mermin and Wagner, which are not related to the glass-transition. These correlations need to be characterized [6] and disentangled from those of $\boldsymbol{C}(\boldsymbol{q},t)$. This makes the project demanding, not only from a computational perspective but also from the theoretical analysis of the simulation data. Apart from the box-size effect, we also plan to consider the effect of confinement (layers, stripes) on the stess correlations and viscoelastic properties of LJ systems.

Profile. The PhD project involves extensive computer simulations and data analysis based on advanced theoretical concepts. The candidate must have a disposition for numerical work and theory. A good background in statistical physics and in programming is required.

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