Proposal for a Master (M2) Internship
2024/2025

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Title : Viscoelastic Memory Functions from Constrained Molecular Dynamics

Background. Many liquids cooled to low temperature do not crystallize, but stay amorphous upon freezing. The amorphous solid is called “glass”. On cooling toward the glass, the viscosity of the liquid increases dramatically. As the viscosity is given by the time-integral of the shear relaxation modulus $G(t)$, this implies that the relaxation of $G(t)$ with time t strongly slows down. Within nonequilibrium statistical mechanics $G(t)$ is defined by the auto-correlation function of the wave-vector ($\boldsymbol{q}$) dependent shear stress in the limit $q \to 0$. A more general quantity is therefore the ($\boldsymbol{q}$,t) dependent correlation function $\boldsymbol{C}(\boldsymbol{q},t)$ of the stress tensor. Recently, $\boldsymbol{C}(\boldsymbol{q},t)$ has attracted a lot of interest for viscoelastic systems, including glassy [1,2] and polymeric liquids [3]. These studies show that $\boldsymbol{C}(\boldsymbol{q},t)$ is determined by “visco-elastic memory functions (VMFs)” encapsulating the interplay of solid-like “elastic” behavior and liquid-like “viscous” flow. The VMFs are thus fundamental quantities that need further analysis. Such analysis, however, is complicated by fact that the VMFs do not evolve with the Newtonian, but with an intricate “constrained” dynamics. This greatly hampers the development of accurate approximations for the VMFs, the quest of which is an active field of research in glass physics [4] and soft matter physics.

Internship project. The complex motion of classical many-body systems can be studied by molecular dynamics (MD) simulations. But, due to the “constrained” dynamics, the VMFs have not been accessible up to now. Our recent work [2] indicates a way to close this gap and may lead to a breakthrough in the field: We argue that the VMFs can be accessed by adding to the MD a force field that is adapted “on the fly” in such a way that constrained dynamics is directly realized in the simulation. Recently, we have made first steps toward implementing this new method in a widely applied HPC (high-performance computing) MD code. We seek a motivated Master student to advance this project, help us create this constrained MD and analyze the ($\boldsymbol{q}$,t) dependent dynamics of viscoelastic liquids. This internship can lead toward a PhD thesis (funding is secured).

Profile. The project involves MD simulations and data analysis based on advanced theoretical concepts. The candidate must have a disposition for numerical work and theory in statistical physics.

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[4] I. Phihlajmaa, V. E. Debets, C. C. L. Laudicina, L. M. C. Janssen, SciPost Physics **15**, 217 (2023).