Potential energy landscape analysis of a supercooled model system under a microrheological perturbation

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We performed molecular dynamics simulations of a binary Lennard-Jones mixture in which an external constant force is applied to one randomly selected particle. In our simulations we observe linear and non-linear responses for the dynamical properties of the driven particle as well as a superdiffusive behaviour along the direction of the applied force for intermediate force strengths and times.

Our analysis is focussed on the time evolution of the system in its potential energy landscape (PEL) which we accessed by explicitly calculating the energetic minima explored by the system. The dynamics of this stationary non-equilibrium system fulfil the general conditions of a continuous time random walk (CTRW) as it was reported for equilibrium systems. In terms of this approach, the dynamical responses can be linked to certain spatial and temporal quantities which allow to identify the relevant contributions to linear and non-linear dynamics.

Additionally, analytical considerations of a CTRW ansatz with an additional force reveal an accessory contribution to the mean square displacement, which can lead to a superdiffusive behaviour in an intermediate time window. These results can be verified by our numerical data.

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