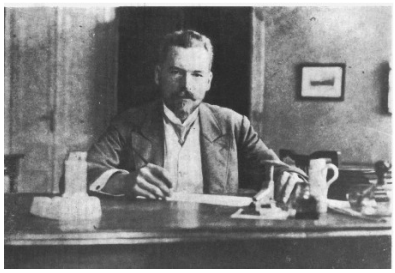

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Short-time molecular motion in simple liquids reflected in temporal, ensemble and wavelet variance MSD for self-diffusion

Thursday, 6 September 2018 09:45 (20 minutes)

The conventional object of interest for studies related to random motions or relatively large walkers in a complex me-dium having traps and obstacles, e.g. biological soft matter that is motivated by a clear separation of scales between their dynamics. On the other hand, molecular motion in simple liquids, where the walker and its surrounding are com-posed of identical particles may exhibit a demonstrable non-Gaussianity as it has been found in the classic Rahman's work on molecular dynamics (MD) simulations of liquid argon. Although the typical time range of this phenomenon is sufficiently shorter than for the self-diffusion coefficient considered thermodynamically, this feature may be closely connected with the behaviour of the macroscopic isochoric heat capacity and the fluctuation theory-based prediction of the liquid density under elevated pressure.

Thus, this work explores MD-based trajectories of molecular motions analysing time, wavelet variance, and ensemble averaged mean-square displacements (MSD). This approach allows for an explicit separation of the characteristic spati-otemporal time scales corresponding to the direct localized intermolecular interactions leading to a sufficiently different ensemble- and single trajectory-based pictures, and the normal ergodic Brownian motion for time scales available for experimental detection. At the same time, there will be discussed, how the characteristics of a microscopic compound process formed by localised fluctuational oscillations and stochastic jumping displacements can be can be accessed from the macroscopic thermodynamic quantities.
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