Collective motion of repulsive Brownian particles in single-file diffusion with and without overtaking

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Particles in dense liquids are hindered from free motion and constantly pushed back by their neighbors, which is often described as a "cage" that confines each particle. The cage effect makes the motion subdiffusive and, in certain cases, eventually leads to the glass transition [1]. The behavior of the mean square displacement (MSD) in dense liquids reflects at least three aspects of the caged dynamics: nearly free motion within the cage for short time, possible drift of the cage enclosing the particle at longer timescale, and hopping of the particle out of the cage as a rare event. Proper characterization of these processes is known to require space-time description, as the cage effect actually emerges from many-body dynamics and involves collective motion, which needs to be captured typically in terms of some four-point space-time correlation [1,2].

In search of methodological insight into theoretical treatment of such collective motions, we have developed a formalism to calculate the displacement correlation of interacting Brownian particles [2,3], in one-dimensional (1D) and two-dimensional (2D) cases, on the basis of the Dean–Kawasaki equation for the fluctuating density field. In the purely 1D case, known as the single-file diffusion (SFD), the theory gives an analytical expression for the displacement correlation [2], which includes the well-known asymptotic behavior of MSD $\propto \sqrt{t}$ as a special case. The 2D theory [3,4] predicts vortical cooperative motion, with negative velocity autocorrelation—a manifestation of the cage effect.

Here we extend the above formalism to SFD with finite interaction potential, allowing the particles to overtake each other as a rare event [5]. By calculating the displacement correlation as an indicator of collective motion, it is shown that overtaking ("hopping") events destroy the short-range correlation, while the long-range weak correlation remains almost intact. Thus we obtain quantitative description of the nested space-time structure of cages, such that small cages are confined in larger cages with longer lifetime.

[l] L. Berthier and G. Biroli, Rev. Mod. Phys. **83**, 587 (2011).

[2] T. Ooshida et al., Phys. Rev. E **88**, 062108 (2013).

[3] T. Ooshida et al., Biophys. Rev. Lett. **11**, 9 (2016).

[4] T. Ooshida et al., Phys. Rev. E **94**, 022125 (2016).

[5] T. Ooshida et al., Mod. Phys. Lett. B **29**, 1550221 (2015).