

The role of hydrodynamics in the diffusion of passive tracers in random networks

Nerea Alcázar-Cano¹, and Rafael Delgado-Buscalioni^{1,2}

¹Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid

²Condensed Matter Physics Center (IFIMAC)

The first natural consequence of the extra reduction in mobility near a wall induced by hydrodynamic interactions (HI) is to decrease the diffusion coefficient. While this statement is true, the role of HI in the diffusion of tracer particles in random media presents other many unexpected faces, some of them still not fully explored. The present study highlights the role of the network structure: we have considered randomly distributed polymeric fibers, cubic networks formed by randomly placed mutually orthogonal rods (Fig. 1 (a) and (b), respectively), and irregular thicker walls formed by colloidal gels. We unveil the relevance of both HI and the obstacle configuration by analysing the “history” of the particle diffusion, evidenced in the van Hove distribution $P(\Delta, t)$ of the tracer jumps Δ after a lag time t .

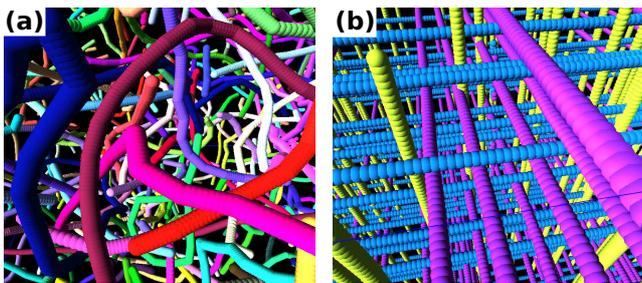


Fig. 1. Pictorial representation of two of our random obstacles structures: (a) polymeric fibrers, and (b) cubic networks.

The details of $P(\Delta, t)$ at long times (or long jumps) subtly depend on the networks structure. We encounter Gaussian tails for $P(\Delta, t)$ in the polymeric network and colloidal gels, while exponential tails in the cubic structure (Fig. 2). Interestingly, all these different behaviours are exclusively due to differences in their *spatial* heterogeneity (the structures are static) [1, 2].

Focusing on hydrodynamics, we find consistently similar hydrodynamic effects in the tracer diffusion across all the random structures considered. As expected, at short times, the probability of small jumps is larger if HI are included (added friction). However at longer times, we observe that the diffusion coefficient of mobile particles in simulations including hydrodynamic interactions (HI) become gradually similar to that of purely Brownian walkers (BD). This HI-induced enhancement of diffusion at long times is more clearly observed close to the critical percolation threshold, i.e., when particles diffuse along single (or very few) fractal paths traversing the system. Our findings suggest that the

origin of the HI-induced enhancement of single-particle diffusion at long times is the anisotropy in the perpendicular and longitudinal tracer mobility close to the obstacle structure. HI induces a faster longitudinal diffusion along the paths, compared with diffusion perpendicular to the obstacle “walls” [3].

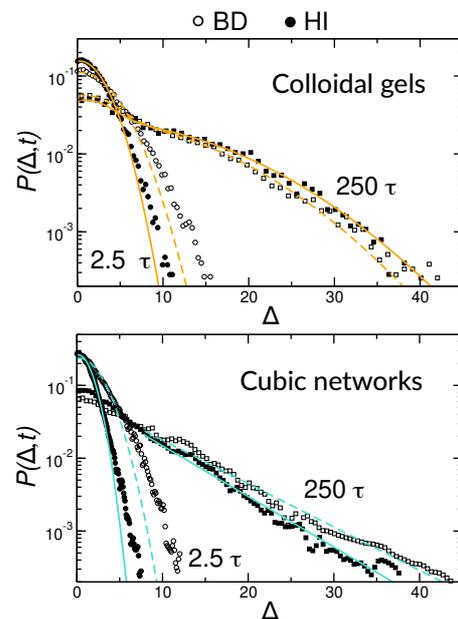


Fig. 2. Displacement probability distribution $P(\Delta, t)$ for a tracer close to the percolation threshold in colloidal gels and cubic networks. Open and filled markers indicate BD and HI simulations, respectively. Lines correspond to different fits: normal distribution at short-time interval ($t = 2.5\tau$), and the combination of two Gaussians in colloidal gels and exponential tails in cubic networks at long time ($t = 250\tau$).

[1] Miotto, J. M., Pigolotti, S., Chechkin, A. V. & Roldán-Vargas, S., *Length scales in Brownian yet non-Gaussian dynamics*, Phys. Rev. X **11**, 031002 (2021).

[2] Skaug, M. J., Wang, L., Ding, Y. & Schwartz, D. K., *Hindered nanoparticle diffusion and void accessibility in a three-dimensional porous medium*, ACS Nano **9**, 21482156 (2015).

[3] Alcázar-Cano, N. & Delgado-Buscalioni, R., *Hydrodynamics induce superdiffusive jumps of passive tracers along critical paths of random networks and colloidal gels*, Soft Matter, DOI: 10.1039/D1SM01713F (2022).