

# Subdiffusion of non-interacting tracers in permanent gels of varying fractal structure

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Porous materials are widely used in a large number of technological applications some of them of daily use. Despite the efforts made over few decades, the mass transport through this kind of materials is not fully understood. In particular, the subdiffusion regime still represents a theoretical challenge. We study the subdiffusion of non-interacting nanoparticles in three-dimensional porous media using Brownian Dynamics. The mean-squared displacement of a particle in this kind of environment presents a power-law time dependence  $\langle r^2 \rangle \propto t^\alpha$ , where  $\alpha$  is the subdiffusive exponent. The diffusive exponent is strongly dependent on tracer diameter  $\sigma$  [1]. As shown in Fig. 1,  $\alpha$  goes to zero as the diffusing particle is larger than some critical value  $\sigma_c$ .

On the other hand, in the gel, the structure of the voids available for the particle to diffuse critically determines its dynamics. The probability of finding an accessible site  $p$  in the percolating void-space of a gel is given by two contributions: the probability of being in the largest percolating void-cluster and that of being in an isolated cluster. Mobile particles diffuse through the percolating cluster while trapped tracers remain in the cages of these isolated spaces (this means that  $\alpha_{\text{trap}} \simeq 0$ ). Of course  $p$  decreases with  $\sigma$  (the relation being different for random obstacles and connected traps).

For a critical void fraction  $p_c$  the percolated void disappears and the diffusion coefficient vanishes [3]. We propose the expression for the subdiffusive exponent

$$\alpha = \alpha_{\text{mob}}(p) [1 - p_{\text{trap}}(p)], \quad (1)$$

which takes into account that, in a fixed gel, a particle is either trapped or mobile ( $1 = p_{\text{mob}} + p_{\text{trap}}$ ). Here  $\alpha_{\text{mob}}$  is the subdiffusive exponent of mobile tracers.

We also propose a simple argument which yields  $\alpha_{\text{mob}} = 1 + a \ln p$ , being  $a$  a parameter which is seen to slightly depends on the gel structure ( $a = 0.20 \pm 0.04$ ). This estimate of  $\alpha$  is compared with our results for several types of gels and also with experimental and numerical works in the literature. We find a fairly good agreement: Figure 2 shows results for  $\alpha$  in two of our gels (a random cubic mesh and polymer gels) and a silica gel studied in Ref. [2]. Solid lines are the fits obtained using Eq. (1). Notably, the probability of getting trapped  $p_{\text{trap}}(p)$  depends on the gel structure. In polymer gels  $p_{\text{trap}} \sim (p/p_c)^{-\gamma}$ , while in cubic and silica gels  $p_{\text{trap}} \sim \exp[-(p/p_c)]$ . Our ansatz also reproduces the subdiffusion observed in actin fibers and random obstacles (Lorentz model).

[2] D. Hlushkou, A. Svidrytski, and T. Ulrich, *J. Phys. Chem. C* **121**, 8416-8426 (2017).

[3] S. Babu, J. C. Gimel, and T. Nicolai, *J. Phys. Chem. B* **112**, 743-748 (2008).

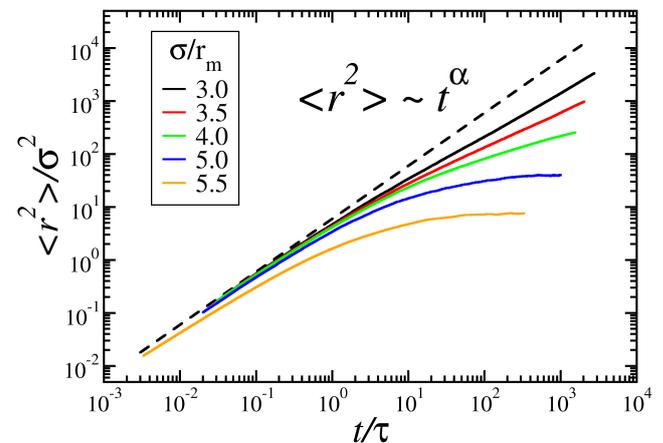


Fig. 1. Mean-square displacement for various particle effective diameter  $\sigma$  in a cubic gel as a function of scale time  $t/\tau$ , where  $\tau$  is the time which a free particle spends on travelling the square of its size. The dashed line represents the dynamics of a free particle, which is purely diffusive  $\langle r^2 \rangle \sim t$ .

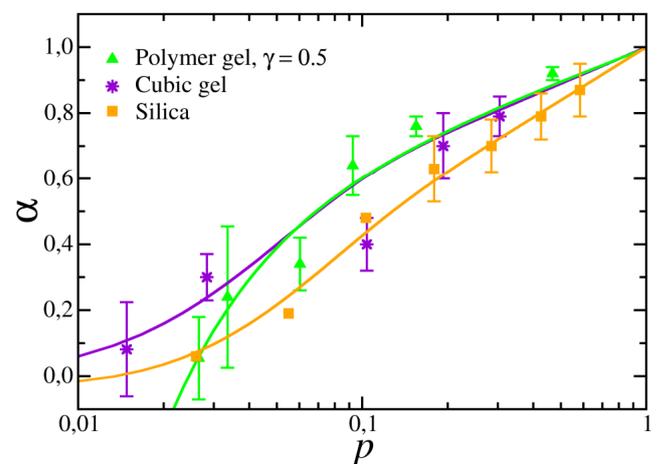


Fig. 2. Subdiffusive exponent  $\alpha$  as a function of the accessible volume fraction  $p$  for three different systems.  $\alpha$  for polymer and cubic gels are the results of our simulations, while silica's results are taking for [2]. Solid lines represent the trend proposed in Eq. (1).

[1] I. Y. Wong, M. L. Gardel, D. R. Reichman, E. R. Weeks, M. T. Valentine, A. R. Bausch, and D. A. Weitz, *Phys. Rev. Lett.* **92**, 178101 (2004).