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Characterization of diffusion processes by the distribution of diffusivities

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Many transport phenomena in physical and biological systems are described by diffusion processes. The observation of individual particles such as tracer molecules offers an interesting approach to characterize the motion by single-particle tracking (SPT). The observed trajectories are typically analyzed by mean-squared displacements. However, this method conceals significant properties of the motion in inhomogeneous systems due to averaging along a trajectory or over an ensemble. Hence, instead of averaging we introduced an analysis which considers diffusivities D defined as scaled squared displacements during a time lag τ along a trajectory in the distribution of diffusivities $p(D,\tau)$ [1]. This distribution describes the diffusivity as a fluctuating quantity and allows further analysis of statistical properties. It should be noted that the first moment of the distribution corresponds to the slope of the well-known mean-squared displacements and identifies the mean diffusion coefficient of the system.

Depending on the nature of the system diffusion is governed by different mechanisms. In heterogeneous systems, such as the two-region exchange model, the diffusion coefficient changes with time. Hence, the distribution of diffusivities depends on the time-lag τ which allows a characterization of the properties of the observed system [2]. In this context we showed how this analysis is closely related to ensemble methods such as pulsed field gradient nuclear magnetic resonance (PFG NMR) providing further benefits.

The distribution of diffusivities also revealed advantages over conventional analysis when observing anisotropic processes where the diffusion coefficient depends on the direction of motion. In such systems the asymptotic decay of the distribution of diffusivities deviates from its first moment [3]. This enables a detection of the anisotropy and even allows a simple reconstruction of the diffusion tensor.

Furthermore, the distribution of diffusivities can also be obtained from an ensemble of particles which coincides with the distribution from a single trajectory for ergodic systems. This is especially interesting for anomalous diffusion, where we extended our concepts to the distribution of generalized diffusivities $p_\alpha(D,\tau)$ which takes the diffusion exponent α into account [4]. In systems showing anomalous diffusion ergodicity can be broken. The most prominent example are subdiffusive continuous time random walks which are known to show interesting phenomena such as aging and weak ergodicity breaking. As a consequence, the distributions of generalized diffusivities which are obtained from ensemble and time averages, respectively, do not coincide (see Fig. 1) and depend in a nontrivial way on the elapsed time between the beginning of the process and the beginning of the measurement. In this context our new analysis tool reveals a deeper understanding of weak ergodicity breaking.

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References

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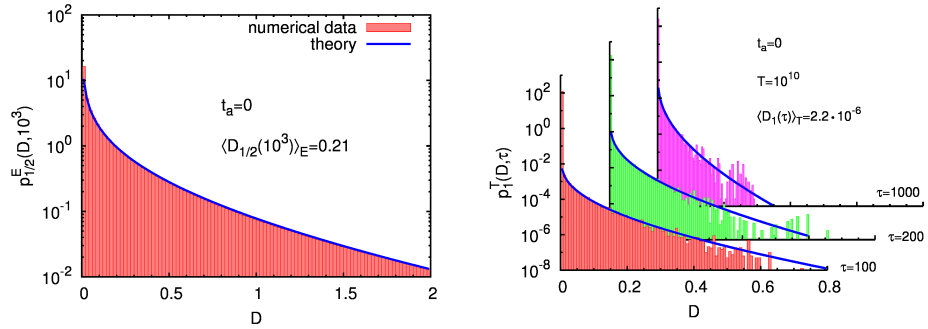

Figure 1: Distribution of generalized diffusivities obtained from an ensemble of subdiffusive continuous time random walk trajectories (left) compared to the distribution which is obtained as time average from only one realization of a subdiffusive continuous time random walk (right). The differences between both distributions, where the left one is asymptotically τ-independent for large τ and the right one shows a strong τ dependence, are obvious and caused by weak ergodicity breaking, which is known to occur in this system.

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