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Characterization of diffusion processes observed with measurement noise by the distribution of diffusivities

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Diffusion is an important mechanism for the transport of particles and molecules in many physical and biological systems. In single-particle tracking (SPT) a characterization of such processes becomes possible by observing the motion of individual tracers. However, an analysis of these trajectories by conventional methods such as mean-squared displacements often conceals the effects of inhomogeneous systems. Hence, we introduced the distribution of diffusivities $p(D,\tau)$ [1], which is easily obtained from SPT experiments and can be related to ensemble-based methods such as pulsed field gradient nuclear magnetic resonance (PFG NMR) [2]. An investigation of the properties of the distribution of diffusivities and its dependence on the time lag τ between snapshots reveals details of the heterogeneities [2] or the anisotropy of the process [3]. Since in experiments the observed positions of a trajectory are always influenced by measurement noise we study such effects on the distribution of diffusivities. As depicted in Fig. 1, large noise can lead to a remarkable change in the behavior of the distribution of diffusivities for small τ but vanishes for increasing τ. This causes a non-trivial τ-dependence of the distribution of diffusivities even for simple systems. We further show how immobile tracers can be exploited to remove contributions of the measurement noise from the distribution of diffusivities, which is highly relevant for experimental data.

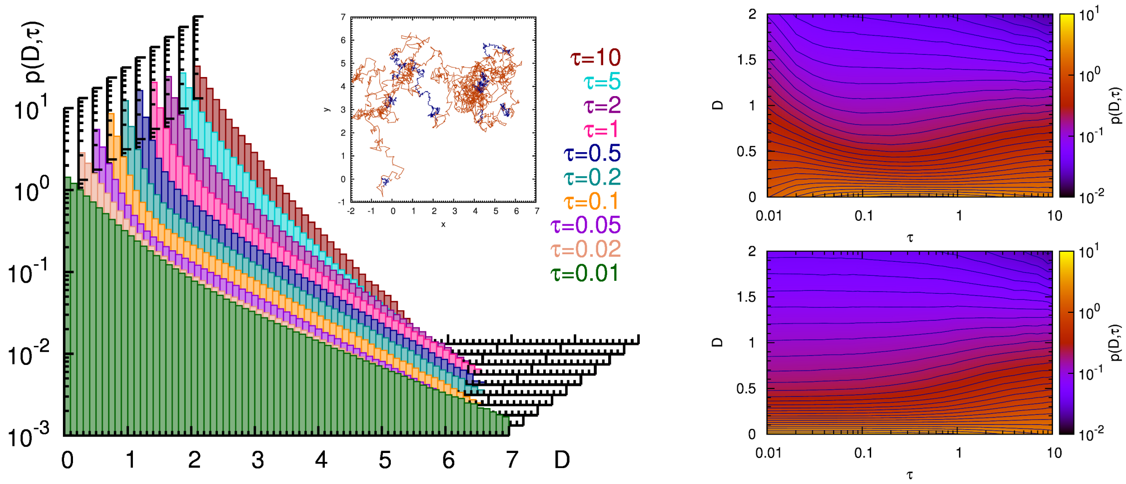

Figure 1: (left) Distributions of diffusivities (histograms) for different time lags τ of a diffusing particle simulated in a bi-layer system [2] where the observed positions are influenced by measurement noise. Both the heterogeneity of the system and the measurement noise govern the decay of the distribution and its convergence to a mono-exponential decay for large τ. The inset shows an example of such a trajectory, where, in contrast to the experiment, information about the layer is color-coded. (right) Comparison of the contour plot of the distributions of diffusivities from the left figure (top) and the same process without additional measurement noise (bottom). For small τ the measurement noise has a large impact on the behavior of the distribution of diffusivities and strongly changes the decay for small diffusivities D. For increasing τ the contribution of the measurement noise vanishes.

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References

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