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Determination of eigenvalues of the diffusion tensor in anisotropic system with spatial orientation change

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By using modern video-microscopic methods, the diffusive motion of individual particles and even molecules can be observed and followed on a sub-micrometer level. The resulting trajectories are analyzed by statistical means in order to obtain the local rheological properties of the surrounding liquid. We already introduced the distribution of diffusivities [1] as a versatile tool for such analysis and showed its utility in the analysis of heterogenous diffusion or by revealing new properties of subdiffusive continuous time random walks [2]. Another possible generalization of homogeneous diffusion processes is anisotropic diffusion. It occurs typically in systems with anisotropic media such as liquid crystals or in isotropic media when the diffusing particle or molecule has an ellipsoidal shape. It can be formally described by an extended Fokker-Planck-equation using a diffusion tensor. We show how the moments of the distribution of diffusivities [3] can be used in a simple fashion to obtain the eigenvalues of the diffusion tensor from trajectories of such anisotropic processes. For a three-dimensional anisotropic system with twist, we show how the method regains the principal diffusion coefficients. In such systems, which are mathematically equivalent to two-dimensional diffusion of an ellipsoid in isotropic media, other methods are harder to accomplish and need better data [4], or might even fail. This can be observed in the figure below, where on the left-hand side the mean squared displacement (MSD) and the angular distribution of displacements did not reveal the anisotropy, whereas on the right-hand side our distribution of diffusivities for the anisotropic system clearly deviates from the isotropic one. In addition, we show for two other systems with spatial orientation change of the diffusion tensor or likewise orientation change of the director, how this affects the distribution of diffusivities. These are a system obeying a Fréedericksz transition and a system which shows undulation of the director.

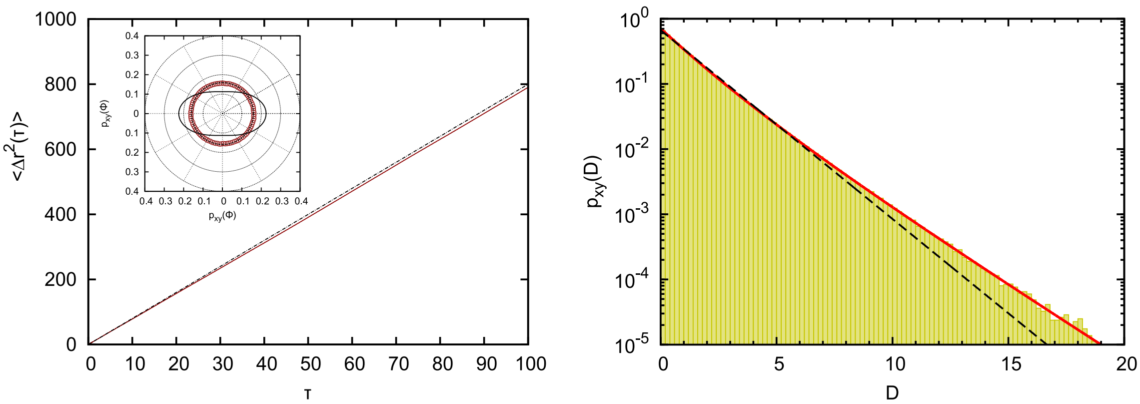

Figure 1: (left) Mean squared displacement of a diffusing ellipsoid (red) and of a diffusing sphere (black dashed) with the same average diffusion coefficient is shown in comparison. The inset shows the angular distribution of the displacements for the ellipsoid (red) and the sphere (black dashed), additionally the angular distribution is shown if the ellipsoid does not rotate (black). (right) The distribution of diffusivities is shown in a logarithmic plot, the yellow bars are the measured distribution, the black dashed line is the expected distribution of a sphere and the red line is the expected distribution of an ellipsoid.

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References

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