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Seminar

Complex Nonlinear Processes in Chemistry and Biology

Honorary Chairman: **G. Ertl**

Organizers: **M. Bär, C. Beta, H. Engel, M. Falcke, M. J. B. Hauser, A. S. Mikhailov, P. Plath, L. Schimansky-Geier, H. Stark**

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Entropic particle transport - higher order corrections to the Fick-Jacobs approach

Abstract

Diffusive transport of particles or, more generally, small objects, is a ubiquitous feature of physical and chemical reaction systems. In microsized geometries with confining walls and constrictions, transport is controlled both by the fluctuations of the jittering objects and the phase space available to their dynamics. For particles moving in static suspension media enclosed by confining geometries and driven by a constant external force, transport exhibits intriguing features such as 1) a decrease in nonlinear mobility with increasing temperature and 2) a broad excess peak of the effective diffusion coefficient above the free diffusion limit. These paradoxical aspects can be understood in terms of entropic contributions resulting from the restricted dynamics in phase space. Assuming instantaneous equilibration in orthogonal channel directions allows for a reduction of the dimensionality of the transport in 2D or 3D channels - the Fick-Jacobs (FJ) approach [1]. Within the resulting 1D kinetic equation the bottlenecks **account for entropic potential barriers which the particles have to overcome in order to proceed. Burada et al. [2] have shown that this approach is only valid for smoothly modulated channel geometries.

In this talk we will present corrections to the Fick-Jacobs approach for more winding channel geometries where the FJ approach usually fails [3]. Two specific geometries exhibiting periodically varying cross-sections are studied in detail, viz., the 3D planar channel and the tube. We employ an asymptotic analysis of the stationary probability density in units of a geometry parameter. This geometry parameter is given by the ratio between the difference of the widest and the most narrow constriction divided through the period length of the channel geometry. We demonstrate that the leading order term is equivalent to the FJ approach. Further we calculate all higher corrections to the stationary probability density. Using these corrections we confirm the expressions for the spatially dependent diffusion coefficient. Especially, we calculate the mean particle current as well as the effective diffusion coefficient for the diffusion dominated transport regime. For example, we find that the averaged velocity and the effective diffusion coefficient are determined by the product of the FJ result for both quantities and the expectation value of the spatially dependent diffusion coefficient for the 3D planar channel geometry. The analytic findings are corroborated with numerical simulations of the particle dynamics in channels with sinusoidal modulated cross-section.

[1]**R. Zwanzig,** ***J. Chem. Phys.*** **p. 3926â3930 (1992)**
[2]**P.S. Burada et. al.,** ***Phil. Trans. R. Soc. A*** **367, p. 3157 - 3171 (2009)**
[3]**S. Martens et. al.,** ***Phys. Rev. E*** **83, 051135 (2011)**

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