Scientific Report for Short Visit Grant 4307
PESC: Exploring the physics of Small Devices (EPSD)

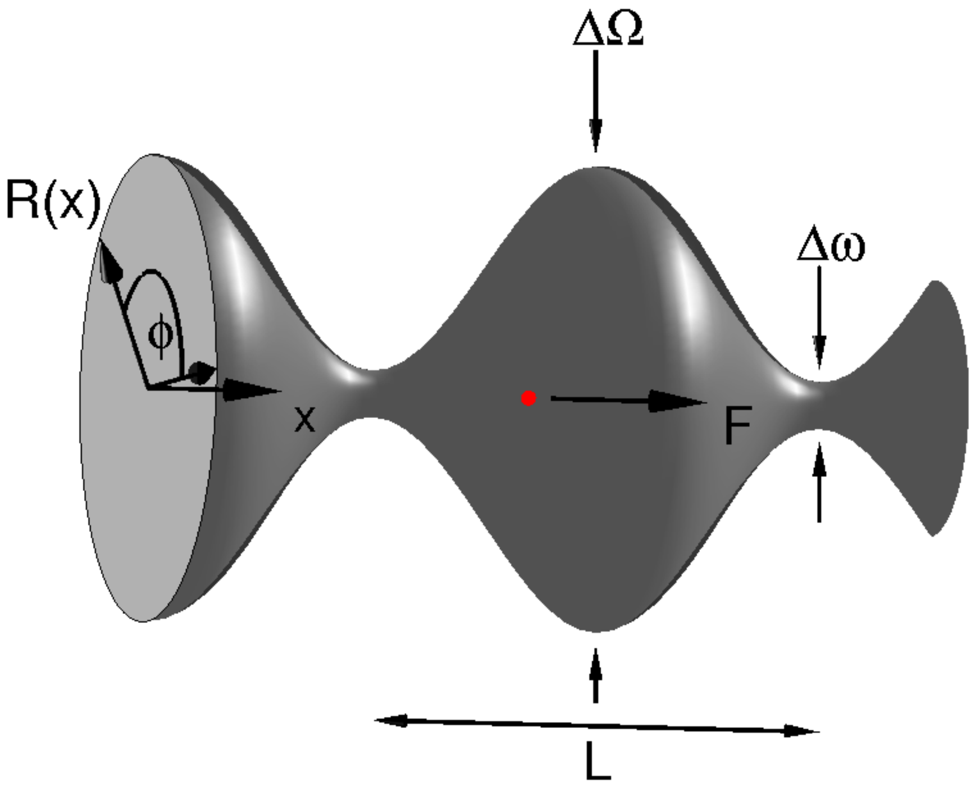
Title of Project: Entropic transport: Corrections to the Fick-Jacobs approximation

Dates of Visit:
Arrival: 06/09/2011 (one day earlier as planned originally)
Departure: 16/09/2011 =11 days

Description of work carried out:

With this visit the PI and the host undertook a study of biased (i.e. with an acting forcing strength F), overdamped Brownian motion of nano-sized objects which takes place within confined, strongly corrugated channel walls. A sketch of the set up is depicted with the figure given below. The bias reflects the action of a static force that acts in transport direction (e.g. of gravitational or electric origin). This problem demands the solution of driven Brownian motion which takes place in a complex 3-d geometry and is complemented with a zero-outflux boundary condition. In order to obtain analytical insight into this three-dimensional, numerically cumbersome problem it is necessary to adopt approximations that reduce dimensionality. We therefore follow the reasoning such as the one used for the conventional Ficks-Jacob approximation scheme for the case of *unbiased* Brownian motion. The key idea is that the problem can then be treated analytically within a one-dimensional approximation along the transport axis for cases when equilibration into the transverse directions occurs on a fast time scale. In doing so, we discussed in our collaboration the use of a mathematical asymptotic expansion in terms of a small parameter which characterizes the strength of the varying geometry along the channel. The scheme is adopted in such a way that in lowest order the usual Ficks-Jacob form, known in the literature, with a characteristic entropic potential is recovered. In particular, we could demonstrate that this estimate is more accurate for extreme corrugated geometries compared to the common applied method. The latter scheme results in a spatially dependent diffusion coefficient D(x, F). We also discussed the option of different choices for the small expansion parameter and whether there exists the possibility for an optimal choice. We believe that no such optimal choice exists.

Open problems:
Apart from extracting explicitly higher order results there is also the open problem how the role of finite inertia affects the findings. We realized that this issue is very complex and not even touched upon in present context for the case of unbiased Brownian motion within confined geometries.



Set up: Sketch of the set up used to study, via an asymptotic expansion method, confined three-dimensional, biased Brownian motion of a nano-sized particle that proceeds along a strongly corrugated channel.

Main results (as of now):
1. Asymptotic diffusion approximation in small parameter that yields in lowest order the Ficks-Jacob-approximation. 2. The next order seemingly is superior to the conventional method using a state-dependent diffusion. 3. Implementation of first simulation results.

Projected publication(s):
The PI's Hänggi and Luczka hope to corroborate the theoretical analysis with extensive numerical simulations. For this latter purpose we are going to collaborate with the group of Professor Schimansky-Geier at Humboldt University where a finite –element program for stochastic dynamics exists and, likewise, with Langevin simulations in an Augsburg-Kattowice collaboration (Dr. Schmid and Dr. Kostur).

Our finalized manuscript is planned to be submitted for publication to either Phys. Rev. E, Eur. Phys. J. B, or possibly also Chaos.