Phase transitions in driven single file diffusion of suspended particles

J. Kurzhals*, **M. Dierl, P. Maass**

Universität Osnabrück, Fachbereich Physik, Barbarastraße 7, 49076 Osnabrück, Germany
*jkurzhals@uos.de

Driven single-file diffusion through channels occurs in many different areas. Important examples are the biased molecular motion through nanotubes or through porous materials with channel-like structures, the incoherent electron transport along molecular wires, the ion transport through membrane channels, and the directed motion of protein motors along filaments. Much work has been devoted in the past to understand anomalous diffusion of tagged particles in single-file transport [1]. With respect to collective properties, phase transitions can be expected to occur based on the findings for the asymmetric simple exclusion process (ASEP) [2].

In this work we study the driven motion of suspended particles of radius R through a two-dimensional narrow channel of width $W<4R$ that is connected to two particle reservoirs, see Fig. 1(a). To this end Brownian dynamics simulations are performed. To cope with the injection of particles into and the ejection of particles from the reservoirs, a special simulation method is implemented based on the bulk-adapted rate method developed in [3,4]. We find that the bulk density of the suspended particles inside the channel exhibits phase transitions as a function of the reservoir densities, reflecting the behavior of the ASEP. According to our coupling to the reservoirs, the phase transitions can be described by applying the minimum and maximum current principles to the current-density relation in a bulk system (channel with periodic boundary conditions), see Fig. 1(b). Possible implications for experiments and applications in microfluidics are pointed out.

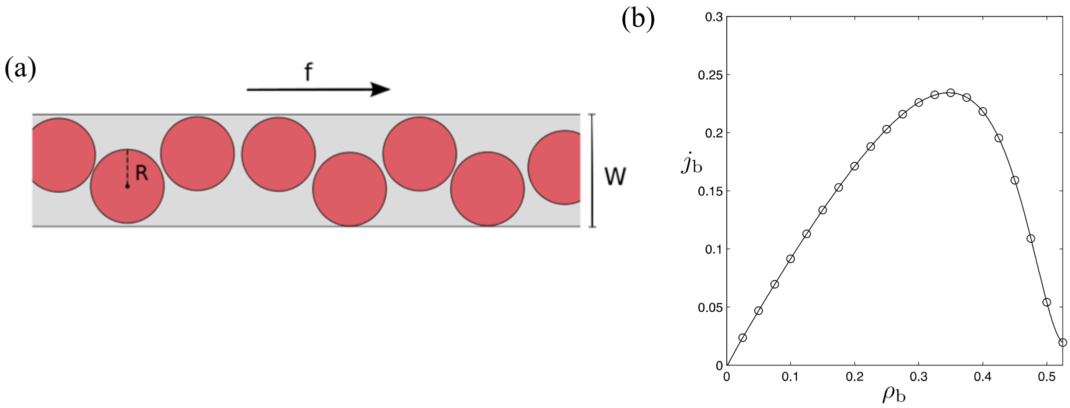

Figure 1: (a) Sketch of suspended Brownian particles that are driven by a force f from a left to a right particle reservoir through a narrow channel of width $W<4R$. (b) Relation between current j_b and density ρ_b in a bulk system (channel with periodic boundary conditions).

References

[1] E. Barkai, R. Silbey; *Theory of single file diffusion in a force field.* Phys. Rev. Lett. **102**, 050602 (2009).

[2] B. Derrida; *An exactly soluble non-equilibrium system: The asymmetric simple exclusion process*. Phys. Rep. **301**, 65-83 (1998).

[3] M. Dierl, P. Maass, M. Einax; *Classical driven transport in open systems with particle interactions and general couplings to reservoirs*. Phys. Rev. Lett. **108**, 060603 (2012).

[4] M. Dierl, M. Einax, P. Maass; *One-dimensional transport of interacting particles: Currents, density profiles, phase diagrams, and symmetries*. Phys. Rev. E **87**, 062126 (2013).

This work is licensed under a Creative Commons Attribution 4.0 International License.
To view a copy of this license, visit http://creativecommons.org/licenses/by/4.0/