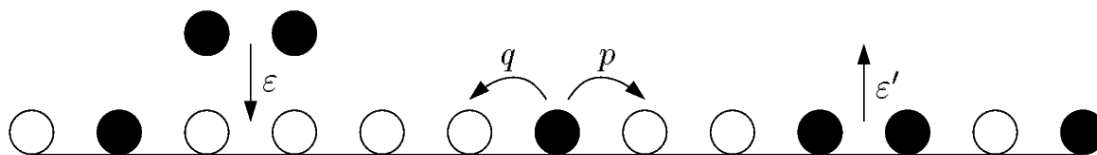


Adsorption-desorption models and catalytic surface processes

Many different complex processes can be modelled mathematically by interacting particle systems. This project will focus on one particular reaction-diffusion model which can be considered as a toy model of catalysis [1] and related by a series of exact mappings to various other systems including some which are experimentally realisable [2].

The model in question is the so-called asymmetric exclusion process (ASEP) combined with deposition and evaporation of dimers (or equivalently pair annihilation and creation) as shown schematically below. The **aim of the project** is to reproduce some known results for this model and then attempt to characterize the distribution of particle currents. Such current fluctuations are a topic of much recent interest in the theory of non-equilibrium statistical mechanics but there are still relatively few cases where they have been calculated exactly [3].



ASEP with dimer evaporation and deposition. Filled circles indicate particles; open circles denote vacancies.

Details.

The asymmetric simple exclusion process (ASEP) is a one-dimensional particle system where random walkers jump preferably in one direction on a lattice and interact via hard-core exclusion. When this process is combined with pair annihilation and creation with particular rates, the model is exactly solvable by a series of mappings to a “free-fermion” system [1]. The first part of the project will be to reproduce analytically the existing results and confirm them by Monte Carlo simulation.

New research progress can then be achieved by studying the current fluctuations in the model within the mathematical framework of large deviation theory [4]. The relevant large deviation function should be accessible analytically (by modifying the stochastic generator) and allow for the testing of certain fluctuation symmetries which are subject to considerable topical attention [5]. A computationally-minded student could also develop algorithms to measure the rare current events in simulations.

Collaboration, prospect for PhD project.

Extensions to the project leading to a possible PhD include the study of typical density profiles conditioning on an extreme particle current and the distribution of defects after a quench of the model parameters. The latter could have particular importance for real catalytic processes and might form part of a collaboration with Dragi Karevski (Institut Jean Lamour, Nancy, France).

The project is jointly supervised by Rosemary Harris, Queen Mary, University of London (QMUL), an expert in non-equilibrium statistical mechanics and fluctuation theorems, and Stefan Grosskinsky, Warwick Complexity. In general, Mathematics in QMUL has a very active research group in statistical mechanics and dynamical systems, with many experts in the area of Complexity Science. Our centre can profit from that expertise, in particular through joint supervision of MSc and PhD students, which we seek to set up in the future.

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