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The Analysis of Interacting Exclusion Processes for Particles of Arbitrary Size: Theoretical and Computational Techniques

Molecular motors are enzymatic molecules that aid many non-equilibrium biological processes such as intracellular transport, translation, etc. These motors carry vesicles ($\geq$ 50 nm) and move with $\sim$ 5nm steps along microtubules. For performing the mechanical work, they convert the chemical energy derived from the hydrolysis of ATP. Experiments reveal that the motor proteins behave cooperatively and interact locally among themselves.

Motivated by the above phenomena, we developed a theoretical framework to analyze the dynamics of interacting oligomers on one-dimensional lattices. We modified the totally asymmetric simple exclusion process (TASEP) describing the unidirectional motion of monomers to include the role of interactions between particles of arbitrary size. We analyzed the periodic as well as the open system using the cluster mean field theory in complement with Monte Carlo simulations. We found that the nature of the current-density relation depends on the strength of interactions, on the size of oligomers and on the way interactions influence particles' transition rates. To explain the dynamic behavior of the system we explicitly obtained the stationary phase diagrams and calculated the particles density correlations for different ranges of parameters. We noticed a good agreement of our theoretical calculations with computer simulations, suggesting that our method correctly describes the main features of the molecular mechanisms of the transport of interacting oligomers.