DY 28: Statistical Physics 5 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)

Time: Tuesday 14:00–15:40   Location: DYb

DY 28.1   Tue 14:00   DYb

Non-Reversible Monte Carlo Simulations of Long-Range Interacting Molecular Systems — ●Philipp Höllmer[1], Liang Qin[2], Michael F. Faulkner[3], A. C. Maggs[4], and Werner Krauth[2] — [1]University of Bonn, Germany — [2]École normale supérieure de Paris, France — [3]University of Bristol, United Kingdom — [4]ESPCI Paris, France

We present current progress of developing non-reversible Markov-chain Monte Carlo (MCMC) algorithms for efficient simulations of atom-based models of molecules that include long-ranged interactions. The event-chain Monte Carlo (ECMC) algorithm samples the Boltzmann distribution exactly without computing energy changes, which removes the computational bottleneck of traditional reversible MCMC simulations. Also, in contrast to molecular dynamics, the mixing and autocorrelation times of MCMC are not locked to the physical dynamics.

We introduce our open-source JeLLyFysh (JF) application that implements ECMC in a general way by demonstrating number of worked out molecular-simulation examples that include, e.g., liquid water. We then highlight recent improvements of the application and ECMC itself. This includes, in particular, the concept of fast sequential Markov chains where ECMC's direction of motion is sequentially chosen from a set. Choosing a large direction set leads to much shorter mixing times of the rotational degree of freedom, and may thus greatly accelerate ECMC simulations of molecular systems.

DY 28.2   Tue 14:20   DYb

What can kinetic Monte Carlo do for active Matter? — ●Juliane U. Klamser[1], Olivier Dauchot[1], and Julien Tailleur[2] — [1]Gulliver UMR CNRS 7083, ESPCI Paris, Université PSL, 75005 Paris, France — [2]Laboratoire Matiere et Systemes Complexes, UMR 7057 CNRS/P7, Université Paris Diderot, 10 rue Alice Domon et Leonie Duquet, 75205 Paris cedex 13, France

As an efficient numerical method, discrete-time, continuous-space Monte Carlo (MC) is wildly used in physics. While constructing an active matter version is straightforward, the question remains to what extent it faithfully captures real-world active systems. We focus on a kinetic MC version for the simplest kind of active matter: persistently moving, non-polar, interacting particles. On the multi-particle level, the MC dynamics captures not only Motility-induced phase separation but also features a non-equilibrium extension of the celebrated two-dimensional melting. An attempt to characterize these phases and their transitions relies on the existence of a thermodynamic pressure, which is not guaranteed outside equilibrium. For a soundly chosen version of the MC dynamics, we show that pressure is a thermodynamic state variable over a robust parameter range. This is demonstrated by deriving the corresponding Langevin description and the associated expression for pressure, which is confirmed by large scale many-particle simulations. Last but not least, our work culminates in a prescription for extending kinetic MC to the standard active matter models, namely active Brownian particles and active Ornstein-Uhlenbeck particles.

DY 28.3   Tue 14:40   DYb

General solution to the one-dimensional connectivity problem — ●Fabian Coupette, Andreas Härtel, and Tanja Schilling — Institut of Physics, University of Freiburg, Germany

We present a general method to obtain the connectivity properties of an arbitrary one-dimensional pairwise interacting n-body system in thermal equilibrium. As input, solely the pair density distribution associated to the equilibrium state is required. Accordingly, if exact analytic results exist for the pair density distribution, the pair connectivity can be determined equally exactly. This is illustrated for fully penetrable and impenetrable rods as well as a repulsive $1/r^2$ nearest-neighbor interaction potential. We also discuss implications of our work for long-ranged interactions, systems in external fields and higher dimensions.

DY 28.4   Tue 15:00   DYb

Criticality in the mechanical regulation of cell adhesion — ●Kristian Blom and Aljaz Godec — Max Planck Institute for Biophysical Chemistry, Göttingen, Germany

Cell adhesion, the process by which cells physically attach to their environment, is established through binding of cellular adhesion molecules located at the outer cell membrane. While on the single molecule level adhesive strength is set by the intrinsic-binding affinity alone, on the many-body level an effective interaction between neighboring adhesion molecules arises through fluctuations of the anchoring cell membrane. Changes in the membrane stiffness, observed in e.g. tumor and muscle cells, alter the effective interaction strength and in turn facilitate mechanical regulation of adhesion. In this talk we will explain how mechanical regulation affects the equilibrium binding state and (un)binding kinetics of adhesion clusters. Ranging from small to large clusters, we show that there always exists an optimal membrane stiffness at which the (un)binding rates are largest. In the thermodynamic limit we observe a dynamical phase transition at which the dominant (un)binding pathway undergoes a qualitative change.

[1] K. Blom, A. Godec, arXiv:2011.05310 (2020)

DY 28.5   Tue 15:20   DYb

Complex routes towards a fully-grown monolayer of "sticky" hard rods — ●Miriam Klopotek, Hans Joachim Schöpe, and Martin Oettel — University of Tübingen, Tübingen, Germany

We study "sticky" hard rods confined to maximally one monolayer, i.e. "(2+1)D" confinement, in a basic, on-lattice model system for thin film growth with anisotropic particles at early stages [1]. We execute a large array of kinetic Monte Carlo (KMC) simulations of the nonequilibrium dynamics [2]. The physics of monolayer growth with "sticky" hard rods is extremely rich. The bounty of phenomena on metastable phases and complex phase transition kinetics we find has not been addressed before by comparable simulation or analytical models. We identify at least five different phase transition scenarios; the different dynamical regimes are traceable in the 2D plane ("map") spanned by the reduced temperature (or attraction strength) and deposition-flux–to–diffusion ratio. The rod-length as well as simple substrate potentials further shift these regimes and alter the topology of the "map", i.e. the set of phase transition scenarios. The specific model choice for microscopic rotational dynamics of rods is another, surprisingly important factor altering the kinetics and, therewith, the morphological evolution.

[1] G. Hlawacek and C. Teichert, *J. Phys.: Condens. Matter* 25 (2013), p. 143202.
[2] M. Klopotek *et al.*, *J. Chem. Phys.* 146.8 (2017), p. 084903.