Phase Transitions In and Out of Equilibrium

Motivated by observations of heterogeneous domain structure on the surface of cells, we consider in the first part of this thesis a minimal model to describe the dynamics of phase separation on the surface of a spherical particle ('meso-sphere'). Our model is given by a two component fluid with a soft repulsive interaction and we describe the evolution of the phase separation with dynamical density functional theory. We consider two different radii of meso-spheres. For the larger meso-sphere we find standard spinodal decomposition, whereas for smaller meso-spheres we observe a long lived metastable state (band state), where two equivalent phases around the poles are separated by the opposite phase around the equator. For the case of a fully phase separated sphere we consider the interaction between a pair of meso-spheres and find that the configuration with the minimal energy cost is obtained when the interfaces between the domains are touching. As a consequence we develop a coarse grained model for spherical particles with an attractive ring around the equator and study their self-assembly behavior. Using Brownian dynamics simulations we find that this kind of interaction leads to the formation of sheet structures.

The methods developed in the first part of the thesis on Brownian dynamics simulations of anisotropic particles are then also used in the second part to investigate the isotropic-nematic transition of self-propelled rods in three dimensions. For this we employ the Gay-Berne interaction potential to model a repulsive ellipsoidal particle. We find that turning on activity moves the phase boundary, separating the isotropic from the nematic phase, to higher densities. This 'active-nematic' phase and its phase boundary are distinct from the boundary between the isotropic phase and polar-clusters which has previously been reported in mainly two dimensional simulation studies. To show that our findings are generic and not sensitive to the precise particle shape or details of interaction we also consider systems of hard spherocylinders and are able to confirm the bend of the isotropic-nematic phase boundary to higher densities as the activity is increased.

For both parts of the thesis, before presenting the result we provide the theoretical and numerical framework used in our calculations.

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