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Summary

This thesis deals with equilibrium and dynamical properties of *colloidal dispersions*. It contains three parts, each concerned with a different colloidal system: in the first part, we present results from classical density functional theory (DFT), dynamical density functional theory (DDFT), and Brownian dynamics (BD) computer simulations on crystallization of a colloidal suspension of paramagnetic spheres on a planar interface that carry a magnetic-field-induced dipole moment, directed perpendicular to the interface. The equilibrium system is completely characterized by the long-range dipole-dipole interactions. The phase behavior is addressed by two different approximations to the DFT, an extended form of the approach by Ramakrishnan and Yussouff (RY) and the extended modified weighted density approximation. Both approaches, which are exact up to third order in the functional expansion of the excess free energy about a fluid with uniform density, are superior to their simpler second-order counterparts. Subsequently, the relaxation dynamics of crystal growth and melting is studied by means of DDFT with the RY density functional as an input and with BD computer simulations. To study the growth scenario, a crystalline cluster of few particles is tagged in an equilibrated fluid at a low magnetic field, before instantaneously increasing the field, which renders the fluid undercooled, and letting the particles free at the same time. Observed is a two-stage process, consisting of a fast relaxation towards a cutout of the stable bulk crystal, which then either collapses or serves as a heterogeneous nucleation seed for further crystal growth, depending on the quench depth and on the structure of the incipient cluster.

The second part deals with crystallization in slit-pore confinement of a model system of particles interacting via ultrasoft repulsive pair potentials representing, e.g., amphiphilic dendrimers in solution, which is addressed with an accurate mean-field DFT and BD computer simulations. The particles are shown to freeze into cluster crystals either from the middle of the slit towards the walls or vice versa, depending on the particle-wall interaction. For large wall-wall separations, a continuous growth of the fluid or solid layer on either wall, upon approaching the bulk freezing line, indicates complete wetting in both cases. The continuous growth is interrupted by capillary melting or freezing.

The third part is devoted to the dynamics of an active, self-propelled, colloidal rod in two dimensions, which serves as a simplified model to study the motion of, e.g., bacteria, spermatozoa, or artificial nano-swimmers close to planar walls. The self-propulsion is modeled through a constant force in the rod orientation and a constant torque, both yielding motion along circles rather than along straight lines; we therefore designate the particle a “Brownian circle swimmer.” The motion in the bulk is examined by integrating analytically the Langevin equations of motion, whereas the motion in linear, confining channels is assessed by a non-Hamiltonian rate theory and BD computer simulations. A sliding mode close to the channel wall leads to a huge acceleration as compared to the bulk motion, which can further be enhanced by an optimum torque-to-force ratio.