



Einladung zum Oberseminar Mathematik in den Naturwissenschaften

Julius-Maximilians-Universität Würzburg
Lehrstuhl für Mathematik in den Naturwissenschaften

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Density functional theory for complex fluids

Classical density functional theory (DFT) is a sophisticated and versatile tool to tackle fundamental physical questions regarding the behavior of various types of equilibrium fluids through a variational principle with respect to the probability density to find a particle at a certain position. The framework of DFT has a deep mathematical foundation provided by a rigorous theorem relating the density of the fluid and the external potential acting on the particles: the knowledge of the density uniquely determines the external potential. In practice, however, the term describing the many-body interaction usually has to be approximated. The most accurate density functionals can be derived for model fluids of hard particles, where the pairwise excluded-volume interaction can be expressed in terms of local measures from integral geometry.

In this seminar, I will give a general introduction to the framework of DFT. Then I present different approaches to make use of DFT within a nonequilibrium context, with the focus on fluids of active Brownian particles. These particles possess an intrinsic self-propulsion mechanism, which can be modeled by a stochastic force introducing memory to the system. Finally, I show some selected results for active particles at interfaces and the phase behavior of hard-body liquid crystals.

Ort: Mathematik Ost, SE40

Zeit: Freitag, 10.01.2020 um 12:00 Uhr

Zu diesem Vortrag sind Sie herzlich eingeladen.

gez. Anja Schlömerkemper