Dynamical density functional theory for orientable colloids including inertia and hydrodynamic interactions

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Abstract-

Over the last few decades, classical density-functional theory (DFT) and its dynamic extensions (DDFTs) have become powerful tools in the study of colloidal fluids. Recently, previous DDFTs for spherically-symmetric particles have been generalised to take into account both inertia and hydrodynamic interactions, two effects which strongly influence non-equilibrium properties. The present work further generalises this framework to systems of anisotropic particles. Starting from the Liouville equation and utilising Zwanzig's projection-operator techniques, we derive the kinetic equation for the Brownian particle distribution function, and by averaging over all but one particle, a DDFT equation is obtained. Whilst this equation has some similarities with DDFTs for spherically-symmetric colloids, it involves a translational-rotational coupling which affects the diffusivity of the (asymmetric) particles. We further show that, in the overdamped (high friction) limit, the DDFT is considerably simplified and is in agreement with a previous DDFT for colloids with arbitrary-shape particles.

Index Terms- Dynamical density functional theory \cdot Colloidal fluids \cdot Arbitrary-shape particles \cdot Orientable colloids

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