Abstract Submitted
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Dynamical density functional theory for arbitrary-shape colloidal fluids including inertia and hydrodynamic interactions[1] MIGUEL A. DURAN-OLIVENCIA, Imperial College London, UK, BEN GODDARD, University of Edinburgh, UK, SERAFIM KALLIADASIS, Imperial College London, UK — Over the last few decades the classical density-functional theory (DFT) and its dynamic extensions (DDFTs) have become a remarkably powerful tool in the study of colloidal fluids. Recently there has been extensive research to generalise all previous DDFTs finally yielding a general DDFT equation (for spherical particles) which takes into account both inertia and hydrodynamic interactions (HI) which strongly influence non-equilibrium properties. The present work will be devoted to a further generalisation of such a framework to systems of anisotropic particles. To this end, the kinetic equation for the Brownian particle distribution function is derived starting from the Liouville equation and making use of Zwanzig's projection-operator techniques. By averaging over all but one particle, a DDFT equation is finally obtained with some similarities to that for spherical colloids. However, there is now an inevitable translational-rotational coupling which affects the diffusivity of asymmetric particles. Lastly, in the overdamped (high friction) limit the theory is notably simplified leading to a DDFT equation which agrees with previous derivations.

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