Phase space dynamical density functional theory for colloids with hydrodynamic interactions

BENJAMIN GODDARD, ANDREAS NOLD, PETR YATSYSHIN, NIKOS SAVVA, Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK, GREG PAVLIOTIS, Department of Mathematics, Imperial College London, London SW7 2AZ, UK, SERAFIM KALLIADASIS, Department of Chemical Engineering, Imperial College London, London SW7 2AZ, UK — We study the dynamics of a colloidal fluid in the full position-momentum phase space. These dynamics are modelled by stochastic equations of motion for a large number of identical spherical particles. We include the full hydrodynamic interactions, which strongly influence the non-equilibrium properties of the system. For large systems, the number of degrees of freedom prohibits a direct solution of the equations and a reduced model is necessary. Under certain assumptions, we derive a dynamical density functional theory (DDFT), i.e. a reduction to the dynamics of the reduced one-body distribution. Our formulation includes the case where the momentum distribution is not a local Maxwellian. Near equilibrium, it reduces to a Navier-Stokes-like equation with additional non-local terms. In the high friction limit, we show rigorously that it reduces to a previously-derived DDFT, describing only the position distribution, but with a novel definition of the diffusion tensor.