

Abstract Submitted
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The effect of the pair correlation function on dynamic density functional theory¹ STEPHEN J. TATE, Department of Chemical Engineering, Imperial College London, BENJAMIN D. GODDARD, School of Mathematics, University of Edinburgh, GRIGORIOS A. PAVLIOTIS, Department of Mathematics, Imperial College London, SERAFIM KALLIADASIS, Department of Chemical Engineering, Imperial College London — In a previous study [1], a general dynamical density functional theory (DDFT) to include hydrodynamic interactions (HI) and inertial effects of colloidal particles was derived and validated with stochastic simulations. But the pair correlation function, g , was approximated with a simplest possible volume-exclusion function, namely a Heaviside step function. Here we explore what effect more accurate g 's have on the same DDFT. These include a correction giving the Percus-Yevick solution for hard spheres, which is known analytically. Furthermore, since we typically deal with systems outside of equilibrium, we model non-adiabatic effects to the HI terms in the DDFT, including density and momentum dependence. [1] B.D. Goddard, A. Nold, N. Savva, G.A. Pavliotis and S. Kalliadasis, "General dynamical density functional theory for classical fluids," *Phys. Rev. Lett.* 109 (120603) 2012.

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