Dynamic density functional theory for nucleation: Non-classical predictions of mesoscopic nucleation theory[1] MIGUEL A. DURAN-OLIVENCIA, PETER YATSYSHIN, Imperial College London, JAMES F. LUTSKO, Université Libre de Bruxelles, SERAFIM KALLIADASIS, Imperial College London — Classical density functional theory (DFT) for fluids and its dynamic extension (DDFT) provide an appealing mean-field framework for describing equilibrium and dynamics of complex soft matter systems. For a long time, homogeneous nucleation was considered to be outside the limits of applicability of DDFT. However, our recently developed mesoscopic nucleation theory (MeNT) based on fluctuating hydrodynamics, reconciles the inherent randomness of the nucleation process with the deterministic nature of DDFT. It turns out that in the weak-noise limit, the most likely path (MLP) for nucleation to occur is determined by the DDFT equations. We present computations of MLPs for homogeneous and heterogeneous nucleation in colloidal suspensions. For homogeneous nucleation, the MLP obtained is in excellent agreement with the reduced order-parameter description of MeNT, which predicts a multistage nucleation pathway. For heterogeneous nucleation, the presence of impurities in the fluid affects the MLP, but remarkably, the overall qualitative picture of homogeneous nucleation persists. Finally, we highlight the use of DDFT as a simulation tool, which is especially appealing as there are no known applications of MeNT to heterogeneous nucleation.

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