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Towards a more accurate microscopic description of the moving contact line problem – incorporating nonlocal effects through a statistical mechanics framework¹ ANDREAS NOLD, Imperial College London, BEN GODDARD, The University of Edinburgh, DAVID SIBLEY, SERAFIM KALLI-ADASIS, Imperial College London — Multiscale effects play a predominant role in wetting phenomena such as the moving contact line. An accurate description is of paramount interest for a wide range of industrial applications, yet it is a matter of ongoing research, due to the difficulty of incorporating different physical effects in one model. Important small-scale phenomena are corrections to the attractive fluid-fluid and wall-fluid forces in inhomogeneous density distributions, which often previously have been accounted for by the disjoining pressure in an ad-hoc manner. We systematically derive a novel model for the description of a single-component liquid-vapor multiphase system which inherently incorporates these nonlocal effects. This derivation, which is inspired by statistical mechanics in the framework of colloidal density functional theory, is critically discussed with respect to its assumptions and restrictions. The model is then employed numerically to study a moving contact line of a liquid fluid displacing its vapor phase. We show how nonlocal physical effects are inherently incorporated by the model and describe how classical macroscopic results for the contact line motion are retrieved.

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