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Canonical density functional theory for hard repulsion

Abstract

Density functional theory has long been established in the grand canonical ensemble (and has met there with great success). The lecture will show how this theory can also be phrased in the canonical ensemble, especially for rigid molecules subject only to hard-core repulsion. By a resummation argument, we shall justify the classical Onsager functional, showing how it should properly be subjected to an additional variational inequality. Much of this work stems from still ongoing discussions with Peter Palffy-Muhoray.