

Density functional theory and the fundamental measure approach to hard spheres fluids in a confining external field

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Master thesis in Soft Matter Physics

Summary of the Master thesis:

Density functional theory (DFT) is a useful tool for studying fluids in any external field. It is used to calculate the density profile in thermal equilibrium and thus other thermodynamical quantities of many systems, like a liquid-gas interface and the resulting surface tension, the structure of a gas inside a box and its thermal compressibility. The quantum version is also used for most of the modern band structure computations in solid state physics. It is thus not limited to the field of soft matter physics but can be formally adapted to many fields related to statistical mechanics.

This work presents the main formalism and mathematical objects of DFT, and shows how it applies to the study of hard spheres fluids in a confining external field. It also presents the Fundamental measure approach used to make proper approximations for DFT in the Hard sphere model, giving results in good agreement with simulations.

The main goal is to compute the density profile and two-body correlation functions of hard rods and hard spheres fluids confined in space by a planar symmetric external potential, showing how the computations are performed and tested. From that the method can be generalized to any other external confinement and the results can be used to compute many interesting thermodynamical quantities.

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