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Contribution ID: **475** Type: **Oral Presentation**

Perturbation Theory for Fluids under Confinement

Thursday, 3 June 2021 19:30 (15 minutes)

Perturbation theory based equations of state (EOS) have the ability to provide insight on the behavior of model fluids, which makes them useful tools in thermodynamics. One of these is the Baker Henderson perturbation theory (BHPT) [1]. It uses the hard sphere fluid as a reference system, and is known to provide accurate predictions for macroscopic pure-component fluids at high temperatures. Small systems are known to deviate from the classical thermodynamic description, which means that a macroscopic EOS will fail to predict the properties of a small system [2]. For fluids confined in small geometries, there is therefore currently a lack of successful methods to predict thermodynamic properties from EOS.

We show how the BHPT can be modified to accurately predict the behavior of fluids under confinement. The extended theory is referred to as BHPT-small. Crucial to this method is the definition of the "bulk"density of a small system, and the behavior of the radial distribution function (RDF). Two major findings were made by investigating how the RDF of a hard sphere fluid, confined by a spherical geometry differs from the bulk RDF. Due to the non-periodic boundaries of the confined system, the RDF will approach zero for at indefinitely pair-distances, instead of tending towards unity. In addition, particles adsorb on the boundary of the spherical confinement, which leads to a depletion of particles in its center. The density experienced by the particles in the center is therefore not equal to the average density of the fluid.

We further demonstrate how BHPT-small can be formulated for pores of different sizes and shapes. The extended perturbation theory provides a tool to compute thermodynamic properties of nanosystems that is applicable to a variety of examples.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

[1] J. A. Barker and D. Henderson. Perturbation theory and equation of state for fluids.
ii. a successful theory of liquids. J Chem Phys, 1967, 47(11), 4714–4721
[2] T. L. Hill. Thermodynamics of Small Systems. J Chem Phys 1962, 36, 3182–3197

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