Soft-core fluid with competing interactions in contact with a hard wall

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Fluids with a pair potential characterized by short-range attraction and long-range repulsion (SALR potential) have been intensively studied for more than a decade and still remain of great interest due to their unusual phase behavior and specific structure properties [1,2]. A SALR potential is of coarse-grained nature and can be used to effectively describe a solvent-mediated interaction between various complex molecules or colloidal particles, such as star-polymers, proteins, grafted nanoparticles, etc. A number of models and corresponding theoretical approaches have been proposed to predict structural and thermodynamic properties of such fluids. However, in most of them the core of fluid particles was considered as strongly repulsive. In our study we focus on a fluid with an interaction, which combines soft core and SALR potentials by representing them in the form of the three-Yukawa potential. The results of Monte Carlo simulations obtained by us show that such a model exhibits microphase separation and clustering phenomena similar to that observed in other SALR models. Moreover, we have noticed that in the case of a fluid confined between two hard walls these phenomena become even more pronounced, e.g. the cluster formation in the confinement can occur at temperatures higher than in the bulk. To understand the effect of confinement in such systems, we aim to develop a field theory approach enabling us to describe a three-Yukawa fluid near a hard wall. As the first step we apply the formalism previously proposed by us for a two-Yukawa fluid [3] and extend it to the case of a three-Yukawa model. At this stage of theory development we restrict our study to the region beyond the cluster formation and verify reliability of our theoretical approach under moderate conditions.

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