

The Smooth Cut-Off Hierarchical Reference Theory of Fluids

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The hierarchical reference theory (HRT) implements the basic concepts of the renormalization group into a microscopic liquid-state approach, and is therefore able to give a realistic treatment of criticality and phase separation, including rigorously flat isotherms in the two-phase region, while also being predictive about the nonuniversal properties of the fluid, which depend on the specific form of the microscopic interaction. However, the implementation of HRT employed so far is plagued by an unphysical divergence of the isothermal compressibility on the whole coexistence curve, thereby forcing it to coincide with the spinodal. We have recently developed a new formulation of the theory, namely the smooth cut-off HRT, which overcomes this limit: on the one hand, the compressibility on the coexistence curve shows the discontinuity expected for a system with a scalar order parameter; on the other hand, the theory also provides a criterion to tell unstable states from metastable ones, hence also giving the location of the spinodal curve. Moreover, for fluids interacting via a hard-core plus attractive Yukawa (HCY) tail, the theory also allows exact enforcement of the requirement that the two-body radial distribution function be vanishing at short distance because of the impenetrable cores. We present results for the thermodynamics and the phase diagram of HCY fluids with several attraction ranges both in and away from the critical region. The present approach is overall at least as accurate as the best liquid-state theories, as shown by the comparison with available simulation data, and goes well beyond them when criticality and phase coexistence come into play.