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Statistical Mechanics Approach for Uniform and Non-uniform Fluid with Hard Core and Interaction Tail

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Abstract: One recently proposed self-consistent hard sphere bridge functional was combined with an exponential function exp(-αr) and a re-normalized indirect correlation function to construct the bridge function for fluid with hard core and interaction tail. In the present approach, the adjustable parameter α was determined by the thermodynamic consistency realized on the compressibility modulus, the re-normalization of the indirect correlation function was realized by a modified Mayer function with the interaction potential replaced by the perturbative part of the interaction potential. As an example, the present bridge function was combined with the Ornstein-Zernike (OZ) equation to predict structure and thermodynamics properties in very good agreement with the simulation data available for Lennard-Jones (LJ). Based on the universality principle of the free energy density functional and the test particle trick, the numerical solution of the OZ equation was employed to construct the first order direct correlation function of the non-uniform fluid as a functional of the density distribution by means of the indirect correlation function. In the framework of the density functional theory, the numerically obtained functional predicted the density distribution of LJ fluid confined in two planar hard walls that is in good agreement with the simulation data.

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Key words: bridge functional, density functional theory, Lennard-Jones fluid

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