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Density Functional Approach Based on Numerically Obtained Bridge Functional

ZHOU Shi-Qi

Research Institute of Modern Statistical Mechanics, Zhuzhou Institute of Technology, Zhuzhou 412008, China
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Abstract: The Ornstein-Zernike equation is solved with the Rogers-Young approximation for bulk hard sphere fluid and Lennard-Jones fluid for several state points. Then the resulted bulk fluid radial distribution function combined with the test particle method is employed to determine numerically the function relationship of bridge functional as a function of indirect correlation function. It is found that all of the calculated points from different phase space state points for a same type of fluid collapse onto a same smooth curve. Then the numerically obtained curve is used to substitute the analytic expression of the bridge functional as a function of indirect correlation function required in the methodology [J. Chem. Phys. 112 (2000) 8079] to determine the density distribution of non-uniform hard sphere fluid and Lennard-Jones fluid. The good agreement of theoretical predictions with the computer simulation data is obtained. The present numerical procedure incorporates the knowledge of bulk fluid radial distribution function into the constructing of the density functional approximation and makes the original methodology more accurate and more flexible for various interaction potential fluid.

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