Structural properties of the Jagla fluid

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The structural properties of the Jagla fluid [1] are studied by Monte Carlo (MC) simulations, numerical solutions of integral equation theories, and the (semi-analytic) rational-function approximation (RFA) method [2, 3, 4].

The Jagla intermolecular pair potential is a spherically symmetric potential consisting of a short-range hard core, a repulsive linear shoulder, and a linear attractive well. It belongs to a family of so-called core-softened potentials and has been invoked to cope with thermodynamic anomalies, such as reentrant melting and the density anomaly, and in connection with liquid-liquid phase transitions in water and other substances [5, 6, 7]. Moreover, the Jagla potential includes as interesting particular cases the ramp and the triangle-well potentials.

The RFA results of the present work [8] are obtained from the assumption (supported by our MC simulations) that the Jagla potential and a potential with a hard core plus an appropriate piecewise constant function lead to practically the same cavity function. The predictions obtained for the radial distribution function $g(r)$ from the RFA method are compared against MC simulations and integral-equation theories for the Jagla model, and also for the limiting cases of the triangle-well potential and the ramp potential, with a general good agreement.

The analytic form of the RFA in Laplace space allows us to describe the asymptotic behavior of $g(r)$ in a clean way and compare it with MC simulations for representative states with oscillatory or monotonic decay, as shown in Fig. 1. The RFA predictions for the Fisher-Widom and Widom lines [9] of the Jagla fluid confirms that this approach is both simple and useful. The RFA produces very reasonable estimates of the damping coefficients for either the monotonic or oscillatory behavior and, in this latter instance, it even leads to an excellent theoretical prediction of the wavelength.

All of the above provides support to the idea that a similar approach to the one followed here for the Jagla fluid may be profitably employed to compute the structural properties of fluids whose molecules interact with other continuous potentials.

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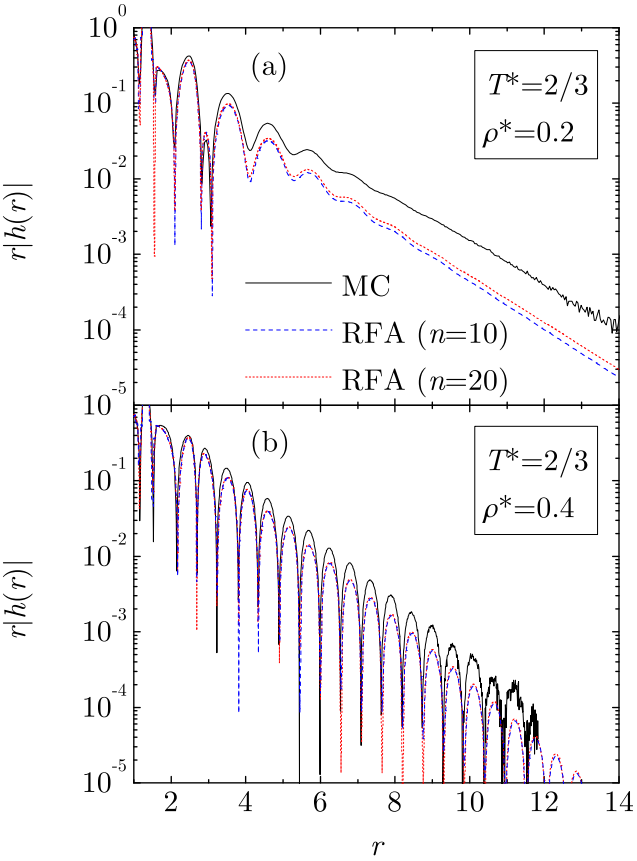

Fig. 1. Semilogarithmic plot of $r|h(r)|$ for a fluid with a Jagla potential ($\lambda_1 = 1.3$, $\lambda_2 = 1.6$, $\epsilon_1/\epsilon_2 = 1$) at (a) $(T^*, \rho^*) = (2/3, 0.2)$ and (b) $(T^*, \rho^*) = (2/3, 0.4)$. The solid, dashed, and dotted lines correspond to MC simulations, and to the RFA with $n = 10$ and $n = 20$ steps, respectively.