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Erratum

Computationally useful bridge diagram series for the structure and thermodynamics of Lennard-Jones fluids

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A trivial error in the coding of the conversion of energy units in the Lennard-Jones potential function used in our recent paper [1] has been found. The equations and theory as well as the molecular dynamics trajectories are unaffected. However, all the analytically calculated bridge functions and dependent thermodynamics are reported as if for a different temperature. Since the convergence properties of the bridge functions with respect to Legendre polynomial order are consistent at all phase points (Fig. 2, Ref. [1]) the relevant discussion is simply corrected by substituting the reduced temperature value $T^* = 7.87$ rather than $T^* = 2.74$.

All affected quantities have been recalculated, and the corrected results for the HNCD2 and HNCD3 in Tables 1 and 2 of the original paper are given here in Tables 1 and 2, respectively. Similar recalculation of the necessary corresponding $\Delta g(r)$ values from Fig. 3a and b of the original paper are given in Fig. 1. The HNC result is unchanged, but is included again for ease of comparison. The corrected thermodynamic values are closer to the simulation results everywhere, which should be expected. In many cases superiority over the PY result is obtained or enhanced. The deviations in the distributions are of the same order of magnitude as in the original paper. There is one difference in the general trends of both the thermodynamics and distribution results. When the interaction potential becomes strongest and the density becomes highest, the HNCD3 result no longer improves the HNCD2 result. This implies that under these extreme conditions the number of significant bridge terms of higher order in density may be large. We also note that the correct bridge diagrams make solution of the equations for HNCD2 and HNCD3 theories possible at all phase points.

Calculations for Sect. 4.3 of the original work have all been rerun with no difference in the (negative) conclusions regarding the use of the functional form of Eq. (28),

Table 1. Excess internal energies per particle, $U^{ex}/N\epsilon$ from the HNCD2 and HNCD3 integral equation theories

$\rho*$	HNCD2	HNCD3
$T^* = 1.35$		
0.70	−4.608	−4.560
0.65	−4.320	−4.286
0.55	−3.700	−3.683
0.50	−3.382	−3.369
0.45	−3.067	−3.056
0.40	−2.759	−2.748
0.35	−2.457	−2.446
0.30	−1.777	−2.148
$T^* = 2.74$		
1.00	−3.383	−3.571
0.80	−3.945	−4.024
0.70	−3.761	−3.807
0.55	−3.159	−3.176
0.40	−2.362	−2.366
0.30	−1.790	−1.791

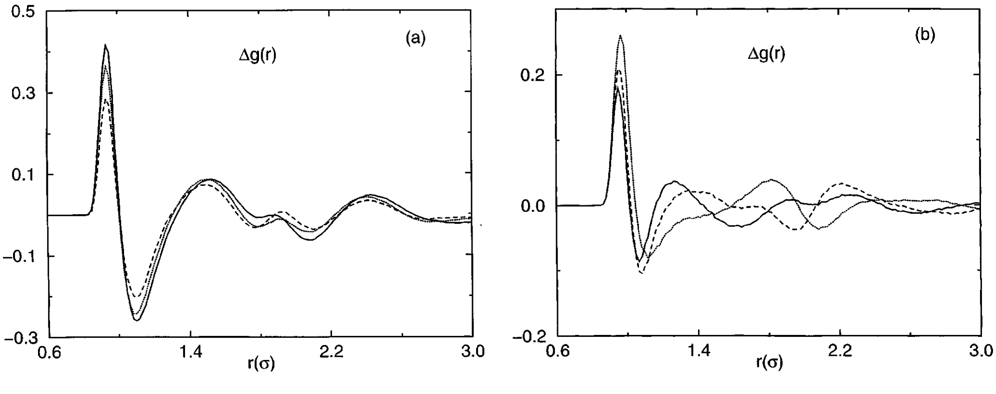

Fig. 1 a The function $\Delta g(r)$, the difference between the result from simulation and each theory. All calculations are for $T^* = 2.74$ and $\rho^* = 1.0$. The *solid line* represents the HNC result, the *dotted line* represents the HNCD2, the *dashed line* is the HNCD3 result. **b** The function $\Delta g(r)$ for $T^* = 2.74$ and $\rho^* = 1.0$. The line types represent the same types of calculations as in **a**

Table 2. Isothermal compressibility factors, $\beta P/\rho$, from the HNCD2 and HNCD3 integral equation theories

$\rho*$	HNCD2	HNCD3
T* = 1.35		
0.70	1.655	1.965
0.65	1.151	1.386
0.55	0.553	0.672
0.50	0.406	0.484
0.45	0.329	0.379
0.40	0.306	0.336
0.35	0.321	0.339
0.30	0.362	0.373
$T*$ = 2.74		
1.00	8.881	8.517
0.80	4.312	4.134
0.70	2.991	2.873
0.55	1.807	1.751
0.40	1.242	1.223
0.30	1.068	1.061

Ref. [1]. Results for the SHNC series sum are still improvements on the HNCD3 thermodynamic results.

Reference

1. Perkyns J, Pettit BM (1997) Theor Chem Acc 96: 61