Erratum: Radial distribution function of penetrable sphere fluids to the second order in density [Phys. Rev. E 75, 021201 (2007)]

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In this paper, we analyzed the radial distribution function of penetrable spheres to the second order in density by exploiting the fact that the individual diagrams in the density expansion are exactly the same as those of hard spheres. We were not able to find the exact analytical expression in the region $0 \leqslant r \leqslant 1$ for the function $\chi(r)$ represented by the only elementary diagram that contributes to the second order. Therefore, several constraints on $\chi(r)$ were derived and a polynomial approximation $\chi_{\text{poly}}(r)$ was proposed for $0 \leqslant r \leqslant 1$ [see Eq. (4.17)]. However, it has been called to our attention that an exact analytical expression was derived long time ago by Ree *et al.* [1]. From their Eq. (19) and making use of the identities

$$\cos^{-1}\frac{2r^2-3}{3} = \cos^{-1}\frac{r^2+r-3}{\sqrt{3(4-r^2)}} + \cos^{-1}\frac{-r^2+r+3}{\sqrt{3(4-r^2)}}, \tag{1}$$

$$\cos^{-1}\frac{r^2-2}{4-r^2} = \cos^{-1}\frac{r^2+r-3}{\sqrt{3(4-r^2)}} - \cos^{-1}\frac{-r^2+r+3}{\sqrt{3(4-r^2)}} \tag{2}$$

one can show that the full expression for $\chi(r)$ is given by Eq. (3.22) with

$$\chi_A(r) = \frac{\pi^2}{630}(r-1)^4(r^2+4r-53-162r^{-1}) - 2\pi\left(\frac{3r^6}{560} - \frac{r^4}{15} + \frac{r^2}{2} - \frac{2r}{15} + \frac{9}{35r}\right)\cos^{-1}\frac{-r^2+r+3}{\sqrt{3(4-r^2)}}. \tag{3}$$

In this paper we checked by comparison with numerical results obtained from Monte Carlo integration that $\chi_{\text{poly}}(r)$ was accurate within six significant figures. To confirm this, Fig. 1 shows a plot of the relative deviation of the polynomial approximation χ_{poly} with respect to the exact function $\chi(r)$. It can be observed that the maximum relative deviation is about 0.8×10^{-6} and occurs at $r \simeq 0.25$.

We are grateful to M. Holovko for calling Ref. [1] to our attention.

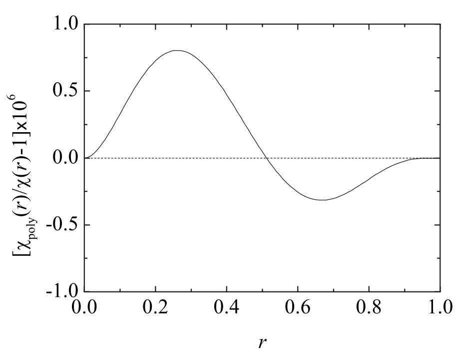

FIG. 1. Relative deviation of the polynomial approximation χ_{poly} with respect to the exact function $\chi(r)$ in the region $0 \leqslant r \leqslant 1$.

[1] F. H. Ree, N. Keeler, and S. L. McCarthy, J. Chem. Phys. **44**, 3407 (1966).

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