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Erratum: "Pair structure of the hard-sphere Yukawa fluid: An improved analytic method versus simulations, Rogers-Young scheme, and experiment" [J. Chem. Phys. 134, 044532 (2011)]

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In a recent paper,[1] we reported on a modified penetrating-background corrected rescaled mean spherical approximation (MPB-RMSA) for the static structure factor of the hard-sphere plus repulsive Yukawa (HSY) fluid. This analytic method is a straightforward modification of the PB-RMSA by Snook and Hayter[2] with improved performance.

In Eq. (17) of Ref. 1 and the related text, we erroneously stated that the modified PB-RMSA consists of replacing the HSY input parameters (k, γ, ϕ) in the PB-RMSA by $(k_{\rm mod}, \gamma, \phi)$, where $k_{\rm mod} = (1-\phi)k$. The correct way of converting the PB-RMSA to the MPB-RMSA is to replace (k, γ, ϕ) by $(k_{\rm mod}, \gamma_{\rm mod}, \phi)$, where

$$k_{\rm mod} = k\sqrt{1-\phi},$$
$$\gamma_{\rm mod} = \gamma \exp(k_{\rm mod}-k)\left(\frac{1+k/2}{1+k_{\rm mod}/2}\right)^2.$$

Accordingly, steps 2–4 of the algorithm described in the Appendix of Ref. 1 must be corrected to

- Step 2:
  Calculate:
  $k_{\rm mod} = k\sqrt{1-\phi}$,
  $\gamma_{\rm mod} = \gamma \exp(k_{\rm mod}-k)\left(\frac{1+k/2}{1+k_{\rm mod}/2}\right)^2$.
- Step 3:
  Assign:
  $k^* = k_{\rm mod} - 2\phi^{1/3}\log(1-\phi)$,
  $\gamma^* = \gamma_{\rm mod}(1-\phi)^{-2}$.
  Determine $g_{\rm MSA}(x=1^+)$, with $x = r/\sigma$, using parameters $[\sigma, \gamma^*, k^*, \phi]$.
  If $g_{\rm MSA}(x=1^+) < 0$, select s from $(0,1)$ and continue with step 4.
  Otherwise assign $\sigma^* = \sigma$ and $\phi^* = \phi$, then go to step 6.
- Step 4:
  Assign:
  $x' = xs$,
  $\sigma^* = \sigma' = \sigma s^{-1}$,
  $\phi^* = \phi' = \phi s^{-3}$,
  $\gamma^* = \gamma'(1-\phi')^{-2} = \gamma_{\rm mod} s(1-\phi')^{-2}$,
  $k' = k_{\rm mod} s^{-1}$,
  $k^* = k' - 2\phi'^{1/3}\log(1-\phi')$.

If step 2 is replaced by $k_{\rm mod} = k$ and $\gamma_{\rm mod} = \gamma$, the original PB-RMSA scheme is recovered. In summary, the modification of the PB-RMSA simply consists of replacing the HSY input parameters (γ, k, ϕ) by $(\gamma_{\rm mod}, k_{\rm mod}, \phi)$.

We point out that all MPB-RMSA results in Ref. 1, as displayed in Figs. 2–11, have been obtained using the correct algorithm given in the present erratum and remain therefore unchanged.

Contrary to what was stated in Ref. 1, Fig. 12 was obtained using the PB-RMSA instead of the MPB-RMSA. Thus, Fig. 12 represents the MPB-RMSA results only when the axis labels $(\tilde{k}, \tilde{T})$ are replaced by $(\tilde{k}_{\rm mod}, \tilde{T}_{\rm mod})$, with

$$\tilde{k}_{\rm mod} = k_{\rm mod}\tilde{d}/\sigma,$$
$$\tilde{T}_{\rm mod} = \exp(\tilde{k}_{\rm mod})/\tilde{\gamma}_{\rm mod}.$$

Here, $\tilde{\gamma}_{\rm mod} = \gamma_{\rm mod}\sigma/\tilde{d}$ and $\tilde{d} = n^{-1/3}$.

The MPB-RMSA diagram in the original $(\tilde{k}, \tilde{T})$ parameter space differs noticeably from the PB-RMSA diagram in Fig. 12 only when both $\tilde{k}$ and ϕ are large. In particular, the inset in Fig. 12 remains practically unchanged and the comparison to the melting line prediction by Bitzer *et al.*[3] is not affected. Moreover, our conclusion regarding the overall superiority of the MPB-RMSA over the PB-RMSA stays intact.

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