

Correction to “Effective Forces in Square Well and Square Shoulder Fluids”

D. Fiocco, G. Pastore, and G. Foffi*

J. Phys. Chem. B **2010**, *114* (37), 12085–12095. DOI: 10.1021/jp105145x

Some mistakes appear in the original version of our paper.¹ Corrections are reported below. Such errors should be regarded as typos, as none of them affect the findings and conclusions of the paper.

1. EQUATION 18

Equation 18 should read

$$2\pi v^2 \int_0^\pi \rho(\mathbf{S}_v; R) \sin \theta \cos \theta \, d\theta \approx \left\langle \frac{1}{dv} \sum_{v < v_i < v+dv} \cos \theta_i \right\rangle \quad (18)$$

2. NUMERICAL VALUES OF $\lambda\sigma_{12}$

The values of $\lambda\sigma_{12}$ used in the paper are

$$\lambda\sigma_{12} = 3.5, 6$$

and not

$$\lambda\sigma_{12} = 3.5, 5.5$$

as stated in the paper.

3. NORMALIZATION OF THE REDUCED FORCE

The definition of the reduced force used in the paper is

$$f_{MC}^*(R) = 2\beta f_{MC}(R)/(\pi\rho\sigma_{11})$$

and not

$$f_{MC}^*(R) = \beta f_{MC}(R)/(\pi\rho\sigma_{11})$$

4. EQUATION 26

Equation 26 should be replaced by the following text:

$$\mathbf{S}_v \equiv \mathbf{s} \quad \text{with } |\mathbf{s}| = v \quad (26)$$

and the use of two new functions ρ' and V' such that

$$\rho(\mathbf{R} + \mathbf{s}) = \rho'(\mathbf{s}) \quad V(\mathbf{R} + \mathbf{s}) = V'(\mathbf{s})$$

has been made, but the prime has been omitted to avoid further cluttering of the notation.

5. EQUATION 31

Equation 31 should read

$$\begin{aligned} {}^1\theta_{\lambda\sigma_{12}} &= \arccos\left(-\frac{R}{2\lambda\sigma_{12}}\right) \\ {}^2\theta_{\lambda\sigma_{12}} &= \arccos\left(\frac{\sigma_{12}^2 - R^2 - \lambda^2\sigma_{12}^2}{2\lambda\sigma_{12}R}\right) \\ {}^1\theta_{\sigma_{12}} &= \arccos\left(\frac{\lambda^2\sigma_{12}^2 - R^2 - \sigma_{12}^2}{2\sigma_{12}R}\right) \\ {}^2\theta_{\sigma_{12}} &= \arccos\left(-\frac{R}{2\sigma_{12}}\right) \end{aligned} \quad (31)$$

■ ACKNOWLEDGMENTS

We acknowledge the help of Guillaume Kon Kam King and Jérémie Breda who pointed out these errors to us.

■ REFERENCES

- (1) Fiocco, D.; Pastore, G.; Foffi, G. *J. Phys. Chem. B* **2010**, *114*, 12085–12095.