

Computer Simulation of Liquids

Michael P. Allen and Dominic J. Tildesley

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List of errata up to May 30, 2018

Line numbers below do not include section headings, equations, figures etc. Negative line numbers are counted up from the bottom of the page.

Chapter 1

p11 $\ell - 16$ ‘It quite possible’ \rightarrow ‘It is quite possible’.

p14 In eqn (1.15) the signs of the odd-order terms are wrong:

$$+T_\alpha \rightarrow -T_\alpha \quad \text{and} \quad +\frac{1}{3}T_{\alpha\beta\gamma} \rightarrow -\frac{1}{3}T_{\alpha\beta\gamma}.$$

F Perez
2017-10-07
MPA
2017-04-04

Chapter 3

p141 In the equation at the top of the page the sign of $\mathbf{r} \cdot \mathbf{f}$ is wrong:

$$\mathcal{P}' = \mathcal{P} + (d/g)\mathbf{p} \cdot \mathbf{p}/m = \frac{1}{dV}(\alpha\mathbf{p} \cdot \mathbf{p}/m + \mathbf{r} \cdot \mathbf{f}) - \frac{\partial\mathcal{V}}{\partial V}.$$

p142 The expression for iL'_2 should have a factor of d :

$$iL'_2 = d(\mathcal{P}' - P)V \frac{\partial}{\partial p_\epsilon}.$$

MPA
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Chapter 4

p162 In the second part of eqn (4.34), defining the terms $\mathcal{V}_m^{(12)}$ and $\mathcal{V}_m^{(6)}$, the negative sign is wrong: $-\mathcal{V}_m^{(6)} \rightarrow +\mathcal{V}_m^{(6)}$, giving

$$\begin{aligned} \mathcal{V}_m &= 4\epsilon \sum_i \sum_{j>i} \left(\frac{\sigma}{L_m s_{ij}^m} \right)^{12} - 4\epsilon \sum_i \sum_{j>i} \left(\frac{\sigma}{L_m s_{ij}^m} \right)^6 \\ &= \mathcal{V}_m^{(12)} + \mathcal{V}_m^{(6)}. \end{aligned}$$

J Mikhail
2018-05-30

Chapter 6

p229 $\ell 8$ ‘charges densities’ \rightarrow ‘charge densities’.

p251 In eqn (6.106) the factor V should be $1/V$:

$$\mathcal{V}_{\text{correction}}^{qq} = \frac{2\pi}{V} \left(\sum_i q_i z_i \right)^2$$

MPA
2017-04-19
J Dürholt
2018-04-13

Chapter 10

p344 In eqn (10.2b) $\int_{r \in A} \rightarrow \int_{r \in B}$.

MPA
2017-03-07