

Computer Simulation of Liquids

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List of errata up to July 30, 2019

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 ℓ –16 ‘It quite possible’ \rightarrow ‘It is quite possible’.

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

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

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

p35 ℓ 11 ‘See Chapter 13’ \rightarrow ‘See Chapter 14’.

MPA
2019-07-30
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p36 ℓ 8 ‘Chapter 5’ \rightarrow ‘Chapter 6’.

p42 ℓ 3 Remove sentence ‘Some of these methods ... Appendix A.’

Chapter 2

p66 ℓ 19, $k_B T/V\beta_T \rightarrow k_B T/V\beta_S$.

MPA & Y Yang
2019-07-22
MPA
2019-07-18

p67 ℓ 8, between eqns (2.85) and (2.86), ‘viral’ \rightarrow ‘virial’.

Chapter 3

p116 All the masses in eqns (3.49ab) should be raised to the power -1 :

A Fleury
2018-08-02

$$\mathbf{r}_{12}(t + \delta t) = \mathbf{r}'_{12}(t + \delta t) + (m_1^{-1} + m_2^{-1})\lambda_{12}^{(r)}\mathbf{r}_{12}(t) - m_2^{-1}\lambda_{23}^{(r)}\mathbf{r}_{23}(t)$$

$$\mathbf{r}_{23}(t + \delta t) = \mathbf{r}'_{23}(t + \delta t) - m_2^{-1}\lambda_{12}^{(r)}\mathbf{r}_{12}(t) + (m_2^{-1} + m_3^{-1})\lambda_{23}^{(r)}\mathbf{r}_{23}(t).$$

The same correction should be applied to eqns (3.53ab); in addition, all the bond vectors in eqns (3.53ab) should be evaluated at $t + \delta t$:

$$\mathbf{v}_{12}(t + \delta t) = \mathbf{v}'_{12}(t + \delta t) + (m_1^{-1} + m_2^{-1})\lambda_{12}^{(v)}\mathbf{r}_{12}(t + \delta t) - m_2^{-1}\lambda_{23}^{(v)}\mathbf{r}_{23}(t + \delta t)$$

$$\mathbf{v}_{23}(t + \delta t) = \mathbf{v}'_{23}(t + \delta t) - m_2^{-1}\lambda_{12}^{(v)}\mathbf{r}_{12}(t + \delta t) + (m_2^{-1} + m_3^{-1})\lambda_{23}^{(v)}\mathbf{r}_{23}(t + \delta t)$$

MPA
2017-04-30

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

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

MPA
2017-04-30

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

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

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

J Mikhail
2018-05-30

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

Chapter 6

p229 ℓ 8 ‘charges densities’ \rightarrow ‘charge densities’.

Also, in eqn (6.43) there is a superfluous right parenthesis in the denominator, should be

MPA
2017-04-19
snafumeander
2019-01-24

$$b(k_x) = \frac{\exp(i(P-1)k_x\ell)}{\sum_{q=0}^{P-2} \exp(ik_x\ell q) M_P(q+1)}.$$

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

J Dürholt
2018-04-13

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

Chapter 10

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

MPA
2017-03-07

Chapter 11

p362 ℓ 6 ‘Fig. 9.4’ \rightarrow ‘Fig. 1.15(b)’.

p379 ℓ –16 ‘Chapter 9’ \rightarrow ‘Chapter 3’.

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2019-07-30
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2019-07-30