

Computer Simulation of Liquids

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List of errata up to August 1, 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

p36 ℓ 8 ‘Chapter 5’ \rightarrow ‘Chapter 6’.

MPA
2019-07-30

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

MPA
2019-07-30

Chapter 2

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

MPA & Y Yang
2019-07-22

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

MPA
2019-07-18

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

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

2017-04-30

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

MPA

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

2017-04-30

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

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

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

J Mikhail
2018-05-30

Chapter 6

- p229** ℓ 8 ‘charges densities’ \rightarrow ‘charge densities’.
Also, in eqn (6.43) there is a superfluous right parenthesis in the denominator, should be

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

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

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

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

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

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

Chapter 13

- p443** ℓ –12 ‘described in Section 13.4’ \rightarrow ‘described in Section 13.2’.
p444 ℓ 9 ‘described in Section 13.4’ \rightarrow ‘described in Section 13.2’.

MPA
2019-08-01
MPA
2019-08-01