Computer Simulation of Liquids
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List of errata up to October 1, 2021

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

F Perez
2017-10-07

p11 ℓ −16 'It quite possible' → 'It is quite possible'.

MPA
2017-04-04

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

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

MPA
2019-08-09

p15 In eqn (1.20), $T_{\alpha\beta} \rightarrow T^{ab}_{\alpha\beta}$. In eqn (1.21), $A_{\alpha\beta} \rightarrow A^{ab}_{\alpha\beta}$.

MPA
2019-08-09

p17 In eqn (1.22), $B_{\alpha\beta} \rightarrow B^{ab}_{\alpha\beta}$, $T_{\alpha\beta} \rightarrow T^{ab}_{\alpha\beta}$, $(\alpha^a)^{-1} \rightarrow (\alpha^a)^{-1}_{\alpha\beta}$.
In eqn (1.23) and ℓ 15, $\tilde{T}_{\alpha\beta} \rightarrow \tilde{T}^{ab}_{\alpha\beta}$. Also in this equation the factor $4\pi\epsilon_0$ should be omitted for consistency with eqn (1.17).

MPA
2019-07-30

p35 ℓ 11 'see Chapter 13' → 'see Chapter 14'.

MPA
2019-07-30

p36 ℓ 8 'Chapter 5' → 'Chapter 6'.

MPA
2019-07-30

p42 ℓ 3 Remove sentence 'Some of these methods … Appendix A.'

Chapter 2

MPA
2019-08-11

p55 In eqn (2.35), $N_n \rightarrow N_c$; in eqns (2.35), (2.36) and ℓ −4, $\mu_n \rightarrow \mu_c$.

MPA & Y Yang
2019-07-22

p66 ℓ 19, $k_\mathrm{B}T/V\beta_T \rightarrow k_\mathrm{B}T/V\beta_S$.

MPA
2019-08-13

p67 ℓ 2, '(eqn (2.82))' → '(eqn (2.62))'.
ℓ 8, between eqns (2.85) and (2.86), 'viral' → 'virial'.

MPA
2019-07-18

Chapter 3

A Fleury 2018-08-02

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

$$\mathbf{r}_{12}(t+\delta t) = \mathbf{r}'_{12}(t+\delta t) + \left(m_1^{-1} + m_2^{-1}\right)\lambda_{12}^{(\mathrm{r})}\mathbf{r}_{12}(t) - m_2^{-1}\lambda_{23}^{(\mathrm{r})}\mathbf{r}_{23}(t)$$
$$\mathbf{r}_{23}(t+\delta t) = \mathbf{r}'_{23}(t+\delta t) - m_2^{-1}\lambda_{12}^{(\mathrm{r})}\mathbf{r}_{12}(t) + \left(m_2^{-1} + m_3^{-1}\right)\lambda_{23}^{(\mathrm{r})}\mathbf{r}_{23}(t).$$

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

$$\mathbf{v}_{12}(t+\delta t) = \mathbf{v}'_{12}(t+\delta t) + \left(m_1^{-1} + m_2^{-1}\right)\lambda_{12}^{(\mathrm{v})}\mathbf{r}_{12}(t+\delta t) - m_2^{-1}\lambda_{23}^{(\mathrm{v})}\mathbf{r}_{23}(t+\delta t)$$
$$\mathbf{v}_{23}(t+\delta t) = \mathbf{v}'_{23}(t+\delta t) - m_2^{-1}\lambda_{12}^{(\mathrm{v})}\mathbf{r}_{12}(t+\delta t) + \left(m_2^{-1} + m_3^{-1}\right)\lambda_{23}^{(\mathrm{v})}\mathbf{r}_{23}(t+\delta t)$$

MPA 2019-08-13

p120 ℓ 14 'eqn (2.161)' $\longrightarrow$ 'eqn (2.167)'.

MPA 2017-04-30 2019-08-21

p141 In the equation at the top of the page the sign of $\mathbf{r}\cdot\mathbf{f}$ is wrong, and a factor $1/dV$ was omitted from the correction term:

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

MPA 2017-04-30

p142 The expression for $\mathrm{i}L'_2$ should have a factor of d:

$$\mathrm{i}L'_2 = d(\mathcal{P}' - P)V\frac{\partial}{\partial p_\varepsilon}.$$

MPA 2019-08-14

p145 In the equations, $T_{\alpha\beta} \longrightarrow T^{ab}_{\alpha\beta}$ and $\left|\mathbf{p}_{\mu^a}\right|^2/m_{\mu^a} \longrightarrow \left|\mathbf{p}_{\mu^a}\right|^2/2m_{\mu^a}$.

Chapter 4

J Mikhail 2018-05-30

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: $-\mathcal{V}_m^{(6)} \longrightarrow +\mathcal{V}_m^{(6)}$, giving

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

Chapter 6

p218 ℓ −4 '(see Fig. 5.6(b))' → '(see Fig. 6.2(b))'. MPA 2019-08-15

p222 Equation (6.16) has the wrong sign: MPA 2019-08-16

$$(\mathbf{f}_{ij})_\alpha = q_i \widehat{T}_{\alpha\beta}\mu_{j\beta} - q_j \widehat{T}_{\alpha\beta}\mu_{i\beta}.$$

p229 ℓ 8 'charges densities' → 'charge densities'. MPA 2017-04-19

Also, in eqn (6.43) there is a superfluous right parenthesis in the denominator, should be snafumeander 2019-01-24

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

p251 In eqn (6.106) the factor V should be $1/V$: J Dürholt 2018-04-13

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

Chapter 9

p333 ℓ 14 '(see Section 4.5)' → '(see Section 4.4)', MPA 2019-08-15

ℓ −2 '(eqn (4.41))' → '(eqn (4.42))'.

p337 ℓ 21 'liquid-vapour' → 'liquid–vapour'. MPA 2019-08-17

Chapter 10

p344 In eqn (10.2b) $\displaystyle\int_{\mathbf{r}\in\mathrm{A}} \to \int_{\mathbf{r}\in\mathrm{B}}$. MPA 2017-03-07

Chapter 11

p360 ℓ −7 'eqn (2.153)' → 'eqn (2.159)'. MPA 2019-08-13

p362 ℓ 6 'Fig. 9.4' → 'Fig. 1.15(b)'. MPA 2019-07-30

p379 ℓ −16 'Chapter 9' → 'Chapter 3'. MPA 2019-07-30

Chapter 13

p420 ℓ −5 'described by eqn (1.36)' → 'described by eqn (1.20)'. MPA 2019-08-10

p443 ℓ −12 'described in Section 13.4' → 'described in Section 13.2'. MPA 2019-08-01

p444 ℓ 9 'described in Section 13.4' → 'described in Section 13.2'. MPA 2019-08-01

Appendix D

MPA
2019-08-19

p502 ℓ −5 ‘eqns (D.1a) and (D.2b)’ → ‘eqns (D.1a) and (D.1b)’.

MPA
2019-08-19

p505 ℓ −5 ‘integral of eqn (D.14a)’ → ‘integral of eqn (D.14b)’.

Appendix E

J Mikhail
2021-09-30

p510 ℓ 12 ‘…generating $X_i = 1$, but allows the possibility of $X_i = 0$;’
→ ‘…generating $\xi_i = 1$, but allows the possibility of $\xi_i = 0$;’.