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

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:

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

Chapter 2

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
2019-07-18

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

Chapter 3

A Fleury
2018-08-02

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

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

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

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

MPA
2017-04-30

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

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

MPA
2017-04-30

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

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

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

MPA
2017-04-19

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

snafumeander
2019-01-24

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

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

J Dürholt
2018-04-13

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

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

Chapter 10

MPA
2017-03-07

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

Chapter 11

MPA
2019-07-30

p362 $\ell 6$ ‘Fig. 9.4’ → ‘Fig. 1.15(b)’.