# *Computer Simulation of Liquids*
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**Second edition, Oxford University Press, 2017**
**List of errata up to August 9, 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** $\ell$ −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 $\ell$ 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** $\ell$ 11 'See Chapter 13' → 'See Chapter 14'.

MPA
2019-07-30

**p36** $\ell$ 8 'Chapter 5' → 'Chapter 6'.

MPA
2019-07-30

**p42** $\ell$ 3 Remove sentence 'Some of these methods … Appendix A.'

## Chapter 2

MPA & Y Yang
2019-07-22

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

MPA
2019-07-18

**p67** $\ell$ 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 $t+\delta t$:

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

**p141** In the equation at the top of the page the sign of $\mathbf{r}\cdot\mathbf{f}$ is wrong: MPA 2017-04-30

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

**p142** The expression for $\mathrm{i}L_2'$ should have a factor of $d$: MPA 2017-04-30

$$\mathrm{i}L_2' = d(\mathcal{P}' - P)V\frac{\partial}{\partial p_\varepsilon}.$$

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

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

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

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

## 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

**p362** $\ell$ 6 'Fig. 9.4' → 'Fig. 1.15(b)'. MPA 2019-07-30

**p379** $\ell$ −16 'Chapter 9' → 'Chapter 3'. MPA 2019-07-30

## Chapter 13

**p443** $\ell$ −12 'described in Section 13.4' → 'described in Section 13.2'. MPA 2019-08-01

**p444** $\ell$ 9 'described in Section 13.4' → 'described in Section 13.2'. MPA 2019-08-01