

# *Computer Simulation of Liquids*

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List of errata up to August 15, 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**  $\ell -16$  ‘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:

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

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

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**p17** In eqn (1.22),  $B_{\alpha\beta} \rightarrow B_{\alpha\beta}^{ab}$ ,  $T_{\alpha\beta} \rightarrow T_{\alpha\beta}^{ab}$ ,  $(\alpha^a)^{-1} \rightarrow (\alpha^a)_{\alpha\beta}^{-1}$ .

In eqn (1.23) and  $\ell 15$ ,  $\tilde{T}_{\alpha\beta} \rightarrow \tilde{T}_{\alpha\beta}^{ab}$ . Also in this equation the factor  $4\pi\epsilon_0$  should be omitted for consistency with eqn (1.17).

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**p35**  $\ell 11$  ‘see Chapter 13’  $\rightarrow$  ‘see Chapter 14’.

**p36**  $\ell 8$  ‘Chapter 5’  $\rightarrow$  ‘Chapter 6’.

**p42**  $\ell 3$  Remove sentence ‘Some of these methods ... Appendix A.’

### Chapter 2

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

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2019-07-22

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

**p67**  $\ell 2$ , ‘(eqn (2.82))’  $\rightarrow$  ‘(eqn (2.62))’.

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

MPA  
2019-08-13  
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  $-1$ :

$$\begin{aligned}\mathbf{r}_{12}(t + \delta t) &= \mathbf{r}'_{12}(t + \delta t) + (m_1^{-1} + m_2^{-1})\lambda_{12}^{(r)}\mathbf{r}_{12}(t) - m_2^{-1}\lambda_{23}^{(r)}\mathbf{r}_{23}(t) \\ \mathbf{r}_{23}(t + \delta t) &= \mathbf{r}'_{23}(t + \delta t) - m_2^{-1}\lambda_{12}^{(r)}\mathbf{r}_{12}(t) + (m_2^{-1} + m_3^{-1})\lambda_{23}^{(r)}\mathbf{r}_{23}(t).\end{aligned}$$

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

$$\begin{aligned}\mathbf{v}_{12}(t + \delta t) &= \mathbf{v}'_{12}(t + \delta t) + (m_1^{-1} + m_2^{-1})\lambda_{12}^{(v)}\mathbf{r}_{12}(t + \delta t) - m_2^{-1}\lambda_{23}^{(v)}\mathbf{r}_{23}(t + \delta t) \\ \mathbf{v}_{23}(t + \delta t) &= \mathbf{v}'_{23}(t + \delta t) - m_2^{-1}\lambda_{12}^{(v)}\mathbf{r}_{12}(t + \delta t) + (m_2^{-1} + m_3^{-1})\lambda_{23}^{(v)}\mathbf{r}_{23}(t + \delta t)\end{aligned}$$

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**p120**  $\ell$  14 ‘eqn (2.161)’  $\rightarrow$  ‘eqn (2.167)’.

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

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

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

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

MPA  
2019-08-14

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

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

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

## Chapter 6

**p229**  $\ell$  8 ‘charges densities’  $\rightarrow$  ‘charge densities’.

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

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

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

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

## Chapter 9

**p333**  $\ell$  14 ‘(see Section 4.5)’  $\rightarrow$  ‘(see Section 4.4)’,  
 $\ell$  -2 ‘(eqn (4.41))’  $\rightarrow$  ‘(eqn (4.42))’.

## Chapter 10

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

## Chapter 11

**p360**  $\ell$  -7 ‘eqn (2.153)’  $\rightarrow$  ‘eqn (2.159)’.

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

**p379**  $\ell$  -16 ‘Chapter 9’  $\rightarrow$  ‘Chapter 3’.

## Chapter 13

**p420**  $\ell$  -5 ‘described by eqn (1.36)’  $\rightarrow$  ‘described by eqn (1.20)’.

**p443**  $\ell$  -12 ‘described in Section 13.4’  $\rightarrow$  ‘described in Section 13.2’.

**p444**  $\ell$  9 ‘described in Section 13.4’  $\rightarrow$  ‘described in Section 13.2’.

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2017-04-19

snafumeander

2019-01-24

J Dürholt

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