Errata for first printing of

Statistical Mechanics: Theory and Molecular Simulation

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The following is a list of the most important corrections to the first printing of the book *Statistical Mechanics: Theory and Molecular Simulation* from Oxford University Press. These and other minor textual corrections are included in the second printing of the book issued in 2010.

Chapter 1

1. Page 2: Two lines below eqn. (1.2.4), there should be no i subscript on the position vectors. They should simply read $\dot{\mathbf{r}} = \mathrm{d}\mathbf{r}/\mathrm{d}t$ and $\ddot{\mathbf{r}} = \mathrm{d}^2\mathbf{r}/\mathrm{d}t^2$.

2. Page 3: The fragmentary sentence in the middle of the page that starts "If the mass falls..." can be fixed by replacing "If" with "Suppose".

3. Page 3: There should be no i index in eqn. (1.2.8). It should read simply

$$\ddot{\mathbf{r}} = 0$$

4. Page 13: In Eq. (1.4.19), there is a factor of 1/2 missing in the second term. The equation should read:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{\beta=1}^{3N} G_{\gamma\beta}(q_1,...,q_{3N})\dot{q}_\beta\right) - \frac{1}{2}\sum_{\alpha=1}^{3N}\sum_{\beta=1}^{3N}\frac{\partial G_{\alpha\beta}(q_1,...,q_{3N})}{\partial q_\gamma}\dot{q}_\alpha\dot{q}_\beta = -\frac{\partial U}{\partial q_\gamma}$$

If we expand out all of the derivatives, note that this equation becomes

$$\sum_{\beta=1}^{3N} G_{\gamma\beta}(q_1,...,q_{3N})\ddot{q}_\beta + \sum_{\alpha=1}^{3N}\sum_{\beta=1}^{3N}\left[\frac{\partial G_{\gamma\beta}}{\partial q_\alpha} - \frac{1}{2}\frac{\partial G_{\alpha\beta}}{\partial q_\gamma}\right]\dot{q}_\alpha\dot{q}_\beta = -\frac{\partial U}{\partial q_\gamma}.$$

Something interesting happens, however, if we try to restore some symmetry to this equation. Note that $\dot{q}_\alpha\dot{q}_\beta$ is symmetric with respect to α and β. Thus, consider rewriting the equation as follows:

$$\sum_{\beta=1}^{3N} G_{\gamma\beta}(q)\ddot{q}_\beta + \frac{1}{2}\sum_{\alpha=1}^{3N}\sum_{\beta=1}^{3N}\left[\frac{\partial G_{\gamma\beta}}{\partial q_\alpha} + \frac{\partial g_{\gamma\alpha}}{\partial q_\beta} - \frac{\partial G_{\alpha\beta}}{\partial q_\gamma}\right]\dot{q}_\alpha\dot{q}_\beta = -\frac{\partial U}{\partial q_\gamma}.$$

where q denotes the full set of generalized coordinates. which is obtained simply by writing

$$
\begin{aligned}
\sum_{\alpha,\beta} \frac{\partial G_{\gamma\beta}}{\partial q_\alpha} \dot{q}_\alpha \dot{q}_\beta &= \frac{1}{2} \sum_{\alpha,\beta} \left[\frac{\partial G_{\gamma\beta}}{\partial q_\alpha} \dot{q}_\alpha \dot{q}_\beta + \frac{\partial G_{\gamma\beta}}{\partial q_\alpha} \right] \dot{q}_\alpha \dot{q}_\beta \\
&= \frac{1}{2} \sum_{\alpha,\beta} \left[\frac{\partial G_{\gamma\beta}}{\partial q_\alpha} \dot{q}_\alpha \dot{q}_\beta + \frac{\partial G_{\gamma\alpha}}{\partial q_\beta} \right] \dot{q}_\alpha \dot{q}_\beta
\end{aligned}
$$

where the last line is obtained simply by interchanging the summation indices in the second term. If we do this, then we obtain the affine connection in the generalized coordinates

$$
\Gamma_{\gamma\beta\alpha} = \frac{1}{2} \left[\frac{\partial G_{\gamma\beta}}{\partial q_\alpha} + \frac{\partial g_{\gamma\alpha}}{\partial q_\beta} - \frac{\partial G_{\alpha\beta}}{\partial q_\gamma} \right] \equiv \frac{1}{2} \left[G_{\gamma\beta,\alpha} + G_{\gamma\alpha,\beta} - G_{\alpha\beta,\gamma} \right]
$$

Finally, if we multiply the equation of motion through by the inverse of the mass-metric tensor, which we will denote here as $G^{\lambda\gamma}$, we obtain the equation of motion in the form (expressed using covariant and contravariant indices) as

$$
\ddot{q}^\lambda + \Gamma^\lambda_{\alpha\beta} \dot{q}^\alpha \dot{q}^\beta = -G^{\lambda\gamma} \frac{\partial U}{\partial q^\gamma}
$$

When $U = 0$, we see manifestly that this becomes the equation of motion for geodesics in the system of curvilinear coordinates.

5. On page 14, the l used to define the areal velocity is not the magnitude of the angular momentum vector discussed below eqn. (1.4.24). To avoid confusion, this l should be replaced by another symbol, say λ, above and in eqn. (1.4.27) and in eqns. (1.4.28) and (1.4.29).

6. On page 20, the dimensionality of the hypersurface is $6N - 1$ not $3N - 1$.

7. Page 33: For consistency, the l subscript in eqn. (1.9.8) should preferably be an i subscript:

$$
\mathbf{a}_{1i} = \frac{1}{2} m_i \dot{\mathbf{r}}_i, \qquad a_{1t} = C
$$

8. Page 35: $\mathbf{F}_\perp$ is a function of $\mathbf{r}$, so a clearer form of eqn. (1.10.2) is

$$
\mathbf{F}_\perp(\mathbf{r}) = [\mathbf{n}(\mathbf{r}) \cdot \mathbf{F}(\mathbf{r})] \, \mathbf{n}(\mathbf{r})
$$

9. Throughout the book, the symbol U is used for the potential energy function. Sec. 1.11 deviates from this convention, so for consistency and clarity, I recommend changing all of the V symbols to U symbols when the potential energy is referenced, as occurs in eqns. (1.11.4), (1.11.5), (1.11.6), (1.11.9), (1.11.21), and (1.11.39).

10. On page 45, the Euler rotation matrix in Eqn. (1.11.42) has errors. The correct matrix is

$$
\mathbf{A}(\theta, \phi, \psi) = \begin{pmatrix} \cos\psi\cos\phi - \cos\theta\sin\phi\sin\psi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\theta\sin\psi \\ -\sin\psi\cos\phi - \cos\theta\sin\phi\cos\psi & -\sin\psi\sin\phi + \cos\theta\cos\phi\cos\psi & -\sin\theta\cos\psi \\ \sin\theta\sin\phi & -\sin\theta\cos\phi & \cos\theta \end{pmatrix}. \tag{1}
$$

11. On page 45, in eqn. (1.11.43), the minus sign in the 12 element of the matrix $\mathbf{A}(\mathbf{q})$ is incorrect. This element of the matrix should be $2(q_2q_3 + q_1q_4)$.

12. On pages 46, the terms eqn. (1.11.44) I_xx, I_yy, and I_zz should be I_{xx}, I_{yy} and I_{zz}.

13. Page 46: On the two lines between eqns. (1.11.45) and (1.11.46), the buried equation $\sum_i = q_i^2 = 1$ should read $\sum_i q_i^2 = 1$.

14. In problem 1.2, the particle should have unit mass ($m = 1$).

Chapter 2

1. Page 67: Four lines below eqn. (2.5.3), the symbol "$\mathrm{x} + t$" should be "x_t".

Chapter 3

1. Page 104: Two lines below eqn. (3.9.5), the constraint functions should be $\sigma_k(\mathbf{r}_1, ..., \mathbf{r}_N)$ and $\dot{\sigma}_k(\mathbf{r}_1, ..., \mathbf{r}_N, \dot{\mathbf{r}}_1, ..., \dot{\mathbf{r}}_N) = \sum_i \nabla_i \sigma_k(\mathbf{r}_1, ..., \mathbf{r}_N) \cdot \dot{\mathbf{r}}_i$.

2. Page 107: The discussion below eqn. (3.9.15) should more precisely be as given below:

   Eqn. (3.9.15) could be used, for example, to obtain $\delta\tilde{\lambda}_1^{(1)}$ followed immediately by an update of all $\mathbf{r}_i^{(1)}$ involved in the $k = 1$ constraint to obtain positions $\mathbf{r}_i^{(2)}$ for this constraint. Given the updated position, eqn. (3.9.15) is used to obtain $\delta\tilde{\lambda}_1^{(2)}$ immediately followed by an update of all $\mathbf{r}_i^{(2)}$ involved in the $k = 1$ constraint, and we iterate until the $k = 1$ constraint is satisfied. We then proceed to the $k = 2$ constraint and iterate until it is satisfied, which will cause a slight violation of the $k = 1$ constraint. Note that satisfying the kth constraint via this procedure causes all $l < k$ constraints to be slightly violated. Thus, after cycling through all of the constraints in this manner, the procedure must be repeated until the full set of constraints is converged to within a given tolerance.

3. Page 114: The bracket is in the wrong place in the last (Lennard-Jones plus Coulomb) term of eqn. (3.11.1). This term should read

$$\sum_{i,j\in\mathrm{nb}} \left\{ 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6} \right] + \frac{q_i q_j}{r_{ij}} \right\}$$

4. On page 117, last line of eqn. (3.11.12), the exponent m should be N.

5. On pages 118-119, the terms eqn. (3.12.6) I_xx, I_yy, and I_zz should be I_{xx}, I_{yy} and I_{zz}.

6. Page 120: In the first line of eqn. (3.13.2), the last term should not have an m in it. The equation for $x(\Delta t)$ should read

$$x(\Delta t) = x(0) + \Delta t \frac{p(0)}{m} - \frac{1}{2}\Delta t^2 \omega^2 x(0)$$

7. Page 121: In the third line from the top of the page, the H should be $\mathcal{H}$, the Hamiltonian.

8. Page 123: In the third line up from Section 3.14, the H should be $\mathcal{H}$, the Hamiltonian.

9. Page 131: In problem 3.5c, the potential should be $U(x) = m\omega^2 x^2/2$. The negative sign is an error.

10. Throughout the chapter, the last name of James Stirling, after whom the Stirling approximation for factorials is named, is misspelled as "Sterling".

Chapter 4

1. Page 133: In the full sentence starting on the fifth line of the second paragraph, each of the three occurrences of the word "constant" should be removed.

2. Page 134: In eqn. (4.2.1), the definition of the chemical potential in the expression on the right is missing a minus sign:

$$\frac{\mu}{T} = -\left(\frac{\partial S}{\partial N}\right)_{V,E}$$

3. Page 154: In the text following Eqn. (4.6.11), the function $g^{(1)}(\mathbf{r})$ should be $(V/N)\rho^{(1)}(\mathbf{r})$, and later $\rho^{(1)} = (N/V)g^{(1)}(\mathbf{r})$. Thus, Eqn. (4.6.12), the integral of $\rho^{(1)}(\mathbf{r})$ should integrate to N:

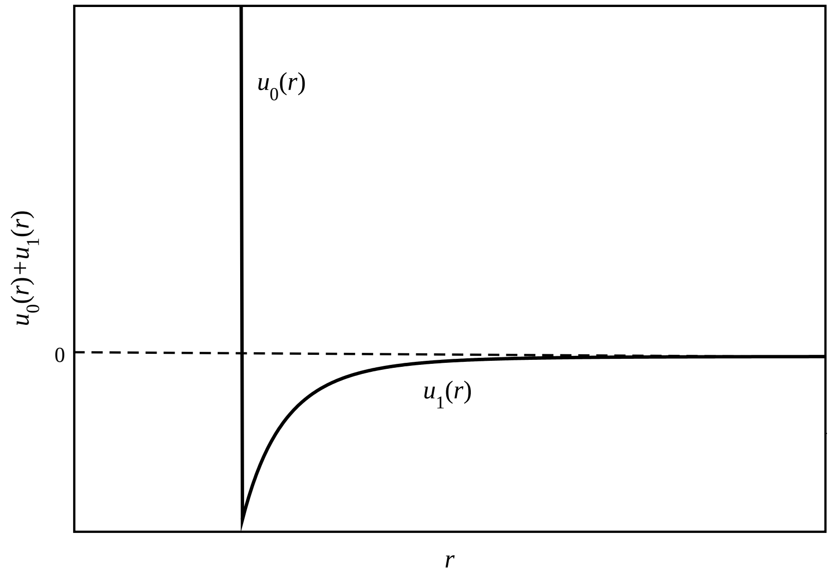
$$\int d\mathbf{r}\ \rho^{(1)}(\mathbf{r}) = N = \frac{N}{V}\int d\mathbf{r}\ g^{(1)}(\mathbf{r}).$$

4. Page 163: The first line of eqn. (4.6.53) should be expressed as a function of the scaled variables as

$$\frac{\partial Z}{\partial V} = \frac{N}{V}Z(N,V,T) - \beta V^N \int d\mathbf{s}_1 \cdots d\mathbf{s}_N \frac{1}{3}V^{-2/3}\left[\sum_{i=1}^{N} \mathbf{s}_i \cdot \frac{\partial U}{\partial(V^{1/3}\mathbf{s}_i)}\right] e^{-\beta U(V^{1/3}\mathbf{s}_1,\ldots,V^{1/3}\mathbf{s}_N)}$$

5. Page 171: In the first line of eqn. (4.7.30), replace the "≈=" simply with "≈".

6. Page 172: In Fig. 4.6, the dashed line representing zero potential energy is in the wrong place. According to the text, $u_1(r) < 0$ for all r and should lie entirely below the dashed line. The figure should, therefore, appear as shown below:



7. Page 176: The last line of eqn. (4.4.47) should read

$$E = -\frac{\partial}{\partial\beta}\left\{\ln\left[\frac{(V-Nb)^N}{N!\lambda^{3N}}\right] + \frac{\beta a N^2}{V}\right\}.$$

   Consequently, two lines below eqn. (4.7.47), the energy should not be the ideal gas result $3NkT/2$ but rather $E = 3NkT/2 - aN^2/V$.

8. Page 181: In eqn. (4.8.13), $f(\mathrm{x})$ is an arbitrary scalar function.

9. Page 182: 9 lines below eqn. (4.8.17), the word "developing" should be "develop", and 4 lines below eqn. (4.8.19), the phrase "of position in sign" should be replaced with "or positive".

10. Page 191: The Q_k in eqn. (4.10.3) should be Q_j. The equation should read

$$\mathcal{H}' = \mathcal{H}(\mathbf{r}, \mathbf{p}) + \sum_{j=1}^{M} \frac{p_{\eta_j}^2}{2Q_j} + dNkT\eta_1 + kT\sum_{j=2}^{M}\eta_j$$

11. Pages 190 and 193: In the captions to Figs. 4.10 and 4.12, the Poincaré sections are generated using the shell $p_\eta \in [-\epsilon, \epsilon]$ for Nosé-Hoover dynamics and $p_{\eta_1}, p_{\eta_2} \in [-\epsilon, \epsilon]$ for Nosé-Hoover chains.

12. Page 197: In eqn. (4.11.17), the product $\prod_{j=M'}^{1}$ is meant to denote a backward product that starts at the $j = M'$ factor and counts down $M' - 1$, $M' - 2$,..., ending at $j = 1$.

13. Page 197-198: The parameter $M' = M - 1$.

14. Page 199: The last operator on the third line of eqn. (4.11.21) has the wrong time step, this operator should be $\exp(iL_{\rm NHC}\delta t/2)$ and not $\exp(iL_{\rm NHC}\Delta t/2)$.

15. Page 199: Some of the subscripts in eqn. (4.11.23) are in correct. The equation should read

$$\sum_{i=1}^{N} \nabla_i \sigma_k \cdot \dot{\mathbf{r}}_i = \sum_{i=1}^{N} \nabla_i \sigma_k \cdot \frac{\mathbf{p}_i}{m_i} = 0.$$

16. Page 200: In the second line of eqn. (4.12.2), the ratio in the prefactor is upside-down. This line should read

$$\frac{Q_{\rm ideal}(N,V,T)}{\Omega_{\rm ideal}(N,V,K)} \mathcal{Q}(N,V,T)$$

17. Page 200: The right side of eqn. (4.12.4) should not contain a sum over i. This equation should read

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_i}\right) - \frac{\partial \mathcal{L}}{\partial \mathbf{r}_i} = \alpha m_i \dot{\mathbf{r}}_i$$

18. Pages 203-205: The K in Eqns. (4.12.3), (4.12.10), (4.12.11), (4.12.14), and (4.12.15) should be $2K$. The same is true in the line just below Eqn. (4.12.10).

19. Page 206: In Eqn. (4.12.23), the position update should be $\mathbf{r}_i \longleftarrow \mathbf{r}_i + \Delta t \mathbf{p}_i/m_i$.

20. Page 213: The second-to-last line on the page should read simply

$$\Gamma(0) = \infty$$

without the $x \leq 0$ condition after it.

Chapter 5

1. Page 219: The $\mathcal{H}$ appearing in eqns. (5.3.6), (5.3.7), and (5.3.8) should be H, which is the enthalpy.
2. Page 219: In the second line of eqn. (5.3.9), the $\mathcal{H}_1(\mathrm{x}_2)$ in the first integral should be $\mathcal{H}_1(\mathrm{x}_1)$.

3. Page 222: The $\mathcal{H}$ in eqns. (5.3.29) and (5.3.30) should be H.

4. Page 228: Some of the summations over γ in eqn. (5.6.11) are out of place or missing. The equation should appear as

$$\begin{aligned}
\langle P^{(\mathrm{int})}_{\alpha\beta}\rangle &= -\frac{kT}{\Delta(N,P,T)}\int \mathrm{d}\mathbf{h}\sum_{\gamma=1}^{3}\frac{\partial}{\partial h_{\alpha\gamma}}\left\{[\det(\mathbf{h})]^{-2}\mathrm{e}^{-\beta P\det(\mathbf{h})}\frac{kT}{\det(\mathbf{h})}h_{\beta\gamma}\right\}Q(N,\mathbf{h},T) \\
&= -\frac{kT}{\Delta(N,P,T)}\int \mathrm{d}\mathbf{h}\sum_{\gamma=1}^{3}\left\{-3[\det(\mathbf{h})]^{-4}\frac{\partial\det(\mathbf{h})}{\partial h_{\alpha\gamma}}h_{\beta\gamma}\right. \\
&\quad \left. -\beta P[\det(\mathbf{h})]^{-3}\frac{\partial\det(\mathbf{h})}{\partial h_{\alpha\gamma}}h_{\beta\gamma}+[\det(\mathbf{h})]^{-3}\frac{\partial h_{\beta\gamma}}{\partial h_{\alpha\gamma}}\right\}\mathrm{e}^{-\beta P\det(\mathbf{h})}Q(N,\mathbf{h},T).
\end{aligned}$$

5. Page 231: The Boltzmann factor at the end of the middle line in eqn. (5.7.16) should be $\exp(-\beta\mathcal{H})$ not $\exp(-\beta H)$.

6. Page 232: In eqn. (5.7.26), the $\beta\gamma$ superscripts on the h in the last line of the equation should be subscripts. The last line of the equation should read

$$\sum_i\sum_\gamma\frac{\partial U}{\partial(\mathbf{h}\mathbf{s}_i)_\alpha}h_{\beta\gamma}s_{i,\gamma}$$

7. Page 234: 8 lines below eqn. (5.8.1), the "$-\partial H/\partial V$" should read "$-\partial\mathcal{H}/\partial V$".

8. Page 237: The first line of eqn. (5.9.2) should read

$$\kappa=\sum_{i=1}^{N}\left[\nabla_{\mathbf{r}_i}\cdot\dot{\mathbf{r}}_i+\nabla_{\mathbf{p}_i}\cdot\dot{\mathbf{p}}_i\right]+\frac{\partial\dot{V}}{\partial V}$$

9. Pages 238 and 241: Eqns. (5.9.5) and (5.10.2) are missing an equation of motion for p_{η_j}, which should read

$$\dot{p}_{\eta_j}=G_j-\frac{p_{\eta_{j+1}}}{Q_{j+1}}p_{\eta_j}$$

10. Page 240: On the line below Fig. 5.3, the definition ξ_c should read $\xi_c=\sum_{k=2}^{M}\xi_k$.

11. Page 244: On the last line of the page, the phrase "isothermal-isoenthalpic" should read "isobaric-isoenthalpic".

12. Page 245: The last term in eqn. (5.12.3) should be dPV. The equation should read

$$G_\epsilon=\alpha\sum_i\frac{\mathbf{p}_i^2}{m_i}+\sum_{i=1}^{N}\mathbf{r}_i\cdot\mathbf{F}_i-dV\frac{\partial U}{\partial V}-dPV$$

13. Page 246: In eqn. (5.12.6), the $\boldsymbol{v}_i(0)$ should be simply $\boldsymbol{v}_i$. Similarly, in eqn. (5.12.8), the $\mathbf{F}_i(0)$ should be simply $\mathbf{F}_i$.

14. Page 250: In eqn. (5.12.26), the $\mathbf{p}_i^2/2m_i$ term in the first line should be $\mathbf{p}_i^2/m_i$.

15. Page 253: On the 7th line from the top, the string of operators should be $\exp(iL_{\epsilon,1}\Delta t)\exp(iL_1\Delta t)\exp(iL_2\Delta t/2)\exp(iL_{\epsilon,2}\Delta t/2)$.

16. Page 253: Four lines below Eqn. (5.13.4), the operator $\exp(iL_t\Delta t)$ should be $\exp(iL_1\Delta t)$.

17. Page 253: In eqn. (5.13.5), the two factors $\mathbf{F}_{c,i}^{(k)(0)}$ in the first and second lines should be $\mathbf{F}_{c,i}^{(k)}(0)$.

18. Page 254: In eqn. (5.13.7), the last factor of $\mathbf{F}_{c,i}^{(k)}(0)$ should be $\mathbf{F}_{c,N}^{(k)}(0)$, so that the equation reads

$$\sigma_l\left(\mathbf{r}_1^{(1)} + \frac{1}{m_1}R_{Fx}(\lambda,0)\sum_k \delta\tilde{\lambda}_k^{(1)}\mathbf{F}_{c,1}^{(k)}(0), ..., \right.$$
$$\left. \mathbf{r}_N^{(1)} + \frac{1}{m_N}R_{Fx}(\lambda,0)\sum_k \delta\tilde{\lambda}_k^{(1)}\mathbf{F}_{c,N}^{(k)}(0)\right) = 0$$

19. Page 255: The string of operators in the unnumbered displayed expression beneath eqn. (5.13.10) should be

$$\exp(iL_{\epsilon,1}\Delta t)\exp(iL_1\Delta t)\exp(iL_2\Delta t/2)\exp(iL_1\Delta t)\exp(iL_{\epsilon,2}\Delta t/2)$$

20. Page 255: In eqn. (5.13.11), the operators on the right side of the equation are in the reverse order. The equation should read:

$$\hat{\mathcal{O}} = \exp(iL_{\mathrm{NHC-baro}}\Delta t/2)\exp(iL_{\mathrm{NHC-part}}\Delta t/2)$$
$$\times \exp(iL_{\epsilon,2}\Delta t/2)\exp(iL_2\Delta t/2).$$

Chapter 6

1. Page 262: In eqn. (6.2.4), the k subscript on the $\partial f/\partial x_k$ factor should be an i subscript, and the equation should read

$$\sum_{i=1}^{k} x_i\frac{\partial f}{\partial x_i} = nf(x_1, ..., x_k, x_{k+1}, ..., x_N)$$

2. Page 263: Just above eqn. (6.2.10), the embedded equation $G(\lambda N, V, T) = \lambda G(N, V, T)$ should read $G(\lambda N, P, T) = \lambda G(N, P, T)$.

3. Page 263: In eqn. (6.3.3), the last term in the last line should be $N\mathrm{d}\mu$, so that this line reads

$$-P\mathrm{d}V - S\mathrm{d}T - N\mathrm{d}\mu$$

4. Page 269: The sentence just after eqn. (6.4.29) should read: "In eqn. (6.4.29), it must be emphasized that the average energy is computed as the derivative with respect to β of $\ln \mathcal{Z}$ at fixed V and ζ *rather* than at fixed V and μ."

Chapter 7

1. Page 291: The ζ_z' at the bottom of the page should be simply ζ_z.

2. Page 299: In eqn. (7.5.4), the functions $f_k(\mathbf{r}^{(K+1)})$ and $f_k(\mathbf{r}^{(K)})$ in the middle line should be $f_K(\mathbf{r}^{(K+1)})$ and $f_K(\mathbf{r}^{(K)})$, respectively, so that this line appears as

$$\min\left[1, \frac{f_K\left(\mathbf{r}^{(K+1)}\right) f_{K+1}\left(\mathbf{r}^{(K)}\right)}{f_K\left(\mathbf{r}^{(K)}\right) f_{K+1}\left(\mathbf{r}^{(K+1)}\right)}\right]$$

3. Page 303: 7 lines from the bottom, the equation "$n\Delta t = t$" should read "$n\Delta t = \mathcal{T}$".

Chapter 8

1. Page 314: 6 lines below eqn. (8.1.6), the word "direction" should be "directly".

2. Page 322: 8 lines above Section 8.4, the acronym "AFD" should be "AFED".

3. Page 325: In the top line, insert the word "satisfies" after "measure".

4. Page 325: In the first line of eqn. (8.4.9), the $Q(N, V, T)$ in the denominator should be $Q_{\mathcal{A}}(N, V, T)$.

5. Page 334: The equation starting at the end of the 5th line from the top and continuing onto the 6th line should read $\delta(\sigma(\mathbf{r})) = \delta(f_1(\mathbf{r}) - s)$.

6. Page 334: At the beginning of the 3rd line following eqn. (8.7.3), the equation is missing a right parenthesis and should read $A(q_{\mathrm{min}}) = 0$.

7. Page 342: In the line just above eqn. (8.8.9), delete the word "applying".

8. Page 344: A "min" is missing in the second line of eqn. (8.9.2).

9. Page 348: In the second line from the bottom of the page, insert the word "need" between "not" and "such".

10. Page 359: In problem 8.9(a), the reference to "problem 4" should be a reference to problem 8.6.

Chapter 9

1. Page 366: The two matrices in eqns. (9.2.10) and (9.2.11) have a few small errors and should appear as

$$\hat{A} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{13} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

$$\hat{A}^{\dagger} = \begin{pmatrix} A^*_{11} & A^*_{21} & A^*_{31} & \cdots \\ A^*_{12} & A^*_{22} & A^*_{31} & \cdots \\ A^*_{13} & A^*_{23} & A^*_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

2. Page 372: 9 lines below eqn. (9.2.39), "Problem 2.5" should be "Problem 2.6".

3. Page 384: 3 lines below eqn. (9.4.4), the $|\psi(m_a;m_b)\rangle$ should be $|\Psi(m_a;m_b)\rangle$.

Chapter 10

1. Page 391: In eqn. (10.1.1), a hat is missing over the $\mathbf{r}_N$. The equation should appear as

$$\hat{\mathcal{H}} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m} + U(\hat{\mathbf{r}}_1, ..., \hat{\mathbf{r}}_N).$$

2. Pages 391 and 392: For consistency with Chapter 11 and for complete generality, the wave functions in eqns. (10.1.4) and (10.1.5) should depend on $\mathbf{x}_1, ..., \mathbf{x}_N$. These equations should appear as

$$\left[-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + U(\mathbf{r}_1, ..., \mathbf{r}_N)\right]\Psi(\mathbf{x}_1, ..., \mathbf{x}_N, t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x}_1, ..., \mathbf{x}_N, t),$$

and

$$\left[-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + U(\mathbf{r}_1, ..., \mathbf{r}_N)\right]\psi_{\{\mathbf{k},m_s\}}(\mathbf{x}_1, ..., \mathbf{x}_N) = E_{\{\mathbf{k},m_s\}}\psi_{\{\mathbf{k},m_s\}}(\mathbf{x}_1, ..., \mathbf{x}_N)$$

respectively.

3. Pages 394 and 395: In eqns. (10.2.13) and (10.2.14), the k subscripts on the ws should all be l subscripts, and the summations should be over l rather than k. These two equations should appear as

$$\begin{aligned}\langle \hat{\mathcal{P}}_{a_k} \rangle &= \mathrm{Tr}(\tilde{\rho}\hat{\mathcal{P}}_{a_k}) \\ &= \sum_l \langle w_l|\tilde{\rho}\hat{\mathcal{P}}_{a_k}|w_l\rangle \\ &= \sum_l w_l \langle w_l|a_k\rangle\langle a_k|w_l\rangle \\ &= \sum_l w_l |\langle a_k|w_l\rangle|^2.\end{aligned}$$

and

$$\frac{1}{\mathcal{Z}}\sum_{\lambda=1}^{\mathcal{Z}} \langle P_{a_k}^{(\lambda)}\rangle = \sum_l w_l |\langle a_k|w_l\rangle|^2$$

In addition, in the paragraph following eqn. (10.2.14), each occurrence of w_k or $|w_k\rangle$ should be w_l or $|w_l\rangle$.

4. Page 400: The minus sign in eqn. (10.4.22) is incorrect and should be deleted.

Chapter 11

1. Page 407: In top line of eqn. (11.2.8), the $(1/\sqrt{L})^{3/2}$ normalization factor should be $(1/L)^{3/2}$.

2. Page 409: The third sentence of Section 11.3 should read "Boltzmann statistics are equivalent to an assumption that the particles are distinguishable because the N-particle wave function for Boltzmann particles is just a simple product of the functions $\phi_{\mathbf{n}_i m_i}(\mathbf{x}_i)$."

3. Page 422: In Eq. (11.5.26), an exponent is missing in the first expression after the equal sign. This part of the expression should read

$$\rho\lambda^3 = \rho\left(\frac{2\pi\hbar^2}{mkT}\right)^{3/2}$$

4. Page 423: In eqn. (11.5.53), the prefactor of $-1/4$ should be $-e^2/4$, where $-e$ is the charge on an electron.

5. Page 424: There should be an e^2 in eqn. (11.5.56). The equation should read

$$C_{\mathrm{x}} = -\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3} e^2$$

6. Page 430: The minus sign between the first and second terms on the right side of eqn. (11.6.10) should be a plus sign:

$$\frac{\rho\lambda^3}{g} = (a_1\rho + a_2\rho^2 + a_3\rho^3 + \cdots) + \frac{1}{2^{3/2}}(a_1\rho + a_2\rho^2 + a_3\rho^3 + \cdots)^2 + \frac{1}{3^{3/2}}(a_1\rho + a_2\rho^2 + a_3\rho^3 + \cdots)^3 + \cdots$$

7. Page 437: In the line just below eqn. (11.6.44), a V subscript is missing in the expression for C_V, and the equation should read $C_V = (\partial E/\partial T)_V$.

Chapter 12

1. Page 445: In the line below Fig. 12.4, insert the word "the" before "number", and in the 7th line below the figure, change "grating" to "gratings".

2. Page 453: In the 5th line above Section 12.3, change "lead" to "leading".

3. Page 465: On the left side of eqn. (12.4.30), the $1/m$ factor should be $m/2$, and the equation should read

$$\int_0^{\beta\hbar} d\tau \frac{m}{2}\dot{y}^2 = \frac{m}{2}\sum_{n=1}^{\infty}\sum_{n'=1}^{\infty} c_n c_{n'}\omega_n\omega_{n'} \int_0^{\beta\hbar} d\tau \cos(\omega_n\tau)\cos(\omega_{n'}\tau).$$

4. Page 470: In eqn. (12.5.9), the argument of U should be $\hat{\mathbf{r}}_1, ..., \hat{\mathbf{r}}_N$, and the equation should read

$$\hat{\mathcal{H}} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m_i} + U(\hat{\mathbf{r}}_1, ..., \hat{\mathbf{r}}_N).$$

5. Page 472: On the second line of eqn. (12.6.2), the fictitious kinetic energy term reads $p_i^2/2m'$, but it should read $p_k^2/2m'$. The entire equation should, therefore, appear as

$$Q_P(L,T) = \int dp_1 \cdots dp_P \int_{D(L)} dx_1 \cdots dx_P \times \exp\left\{-\beta\sum_{k=1}^{P}\left[\frac{p_k^2}{2m'} + \frac{1}{2}m\omega_P^2(x_{k+1}-x_k)^2 + \frac{1}{P}U(x_k)\right]\right\}\Bigg|_{x_{P+1}=x_1}.$$

6. Page 477: In eqn. (12.6.23), the summation in the exponential should range from $k = 1$ to P. The equation should read

$$W(u_1) = -kT \ln \left\{ \int \mathrm{d}u_2 \cdots \mathrm{d}u_P \right.$$
$$\left. \times \exp\left[-\beta \sum_{k=1}^{P} \left(\frac{1}{2} m_k \omega_P^2 u_k^2 + \frac{1}{P} U(x_k(u)) \right) \right] \right\}$$

(Remember that $m_1 = 0$.)

7. Page 478: In eqn. (12.6.24), the fictitious kinetic energy term in the middle line of the equation should have a (k) superscript rather than an (s) superscript. This equation should read

$$Q_P(N,V,T) = \prod_{i=1}^{N} \left(\frac{m_i P}{2\pi\beta\hbar^2} \right)^{dP/2} \int \prod_{i=1}^{N} \mathrm{d}\mathbf{r}_i^{(1)} \cdots \mathrm{d}\mathbf{r}_i^{(P)} \mathrm{d}\mathbf{p}_i^{(1)} \cdots \mathrm{d}\mathbf{p}_i^{(P)}$$

$$\times \exp \left\{ -\beta \sum_{k=1}^{P} \left[\sum_{i=1}^{N} \frac{\mathbf{p}_i^{(k)^2}}{2m_i'} + \sum_{i=1}^{N} \frac{1}{2} m_i \omega_P^2 \left(\mathbf{r}_i^{(k+1)} - \mathbf{r}_i^{(k)} \right)^2 \right. \right.$$

$$\left. \left. + \frac{1}{P} U\left(\mathbf{r}_1^{(k)}, ..., \mathbf{r}_N^{(k)} \right) \right] \right\}$$

Three lines below the equation, replace "index s" with "index k".

8. Page 478: In eqn. (12.6.25), the two (s) super scripts on $\mathbf{p}_i^{(s)}$ and $\mathbf{u}_i^{(s)}$ should be (k) superscripts, and the equation should read

$$\mathcal{H} = \sum_{k=1}^{P} \left[\sum_{i=1}^{N} \frac{\mathbf{p}_i^{(k)^2}}{2m_i^{(s)'}} + \sum_{i=1}^{N} \frac{1}{2} m_i^{(k)} \omega_P^2 \mathbf{u}_i^{(k)^2} + \frac{1}{P} U\left(\mathbf{r}_1^{(k)}(\mathbf{u}_1), ..., \mathbf{r}_N^{(k)}(\mathbf{u}_N) \right) \right].$$

9. Page 480: In Eq. (12.6.26), x_{l+j} on the right side of the equation should be x_{l+k}, so that the equation reads

$$u_{l+k} = x_{l+k} - \frac{kx_{l+k+1} - x_l}{(k+1)} \qquad k = 1, ..., j.$$

10. Page 482: In eqn. (12.6.33), an x_i appears twice and should be x_k. The equation should read

$$\frac{P}{2\beta} - \left\langle \frac{1}{2} m\omega_P^2 \sum_{k=1}^{P} (x_k - x_{k+1})^2 \right\rangle_f = \left\langle \frac{1}{2P} \sum_{k=1}^{P} x_k \frac{\partial U}{\partial x_k} \right\rangle_f.$$

11. Page 483: In eqn. (12.6.39), in the first line of the equation, there is an extra summation $\sum_{k=1}^{P}$ that should be removed, and there is a factor of $\mathrm{e}^{-\beta\alpha(x_1,...,x_P)}$ missing in the second line of the equation. The entire equation should read

$$
\begin{aligned}
\langle \alpha \rangle_f &= \frac{1}{2\beta Q_P} \int \mathrm{d}x_1 \cdots \mathrm{d}x_P \; \mathrm{e}^{-\beta\alpha(x_1,\ldots,x_P)} \sum_{k=1}^{P} \frac{\partial}{\partial x_k} \left[x_k \mathrm{e}^{-\beta\gamma(x_1,\ldots,x_P)} \right] \\
&= \frac{1}{2\beta Q_P} \int \mathrm{d}x_1 \cdots \mathrm{d}x_P \left[P - \frac{\beta}{P} \sum_{k=1}^{P} x_k \frac{\partial U}{\partial x_k} \right] \mathrm{e}^{-\beta\gamma(x_1,\ldots,x_P)} \mathrm{e}^{-\beta\alpha(x_1,\ldots,x_P)} \\
&= \frac{P}{2\beta} - \left\langle \frac{1}{2P} \sum_{k=1}^{P} x_k \frac{\partial U}{\partial x_k} \right\rangle_f ,
\end{aligned}
$$

Chapter 13

1. Page 493: In the line just above eqn. (13.1.2), insert the word "force" after "driving".
2. Page 503: Eqn. (13.3.8) is missing a $2m_i$ factor in the denominator of the first term. The conserved quantity is actually:

$$
\mathcal{H}' = \sum_{i=1}^{N} \frac{1}{2m_i} \left(\mathbf{p}_i + m_i \gamma y_i \hat{\mathbf{e}}_x \right)^2 + U(\mathbf{r}_1, ..., \mathbf{r}_N).
$$

3. Page 506: In the second line below Eqn. (13.3.26), the expression $\mathbf{C}_i(\mathbf{r}, \mathbf{p}) = 1$ should be $\mathbf{C}_i(\mathbf{r}, \mathbf{p}) = 0$.

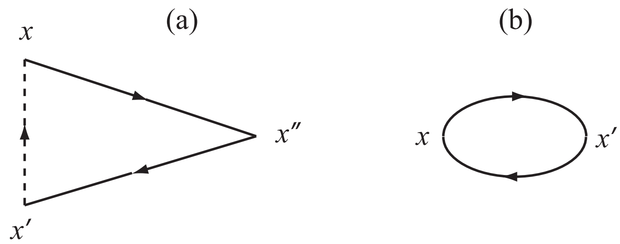
4. Page 511: In the paragraph beginning, "Suppose a molecular dynamics...", the $\mathrm{x}_{n\Delta t}, n = 1, ..., M$ in the second line should be $\mathrm{x}_{m\Delta t}, m = 1, ..., M$. In the fifth line, $\mathrm{x}_0, ..., \mathrm{x}_{K\Delta t}$ should be $\mathrm{x}_1, ..., \mathrm{x}_{K\Delta t}$, and $n = 1, ..., K$ in eqn. (13.4.3) should be $n = 0, ..., K$.

5. Page 515: In the 10th line after eqn. (13.5.1), change the word "longer" to "smaller".

Chapter 14

1. Page 527: 6 lines below eqn. (14.1.1), the fields $E_x(\mathbf{r})$, $E_y(\mathbf{r})$, $E_z(\mathbf{r})$, $B_x(\mathbf{r})$, $B_y(\mathbf{r})$, $B_z(\mathbf{r})$ should be $E_x(\mathbf{r}, t)$, $E_y(\mathbf{r}, t)$, $E_z(\mathbf{r}, t)$, $B_x(\mathbf{r}, t)$, $B_y(\mathbf{r}, t)$, $B_z(\mathbf{r}, t)$.

2. Page 555: Eqn. (14.6.3) is not consistent with the explanation that follows nor with Fig. 14.6. The sentence "Starting at x...." in the paragraph following eqn. (14.6.3) should be replaced with "Starting at x, propagate along a real-time path to the point x'' using the propagator $\exp(-i\hat{\mathcal{H}}t/\hbar)$ and evaluate the eigenvalue $b(x'')$ of $\hat{B}$ at that point; from x'', propagate backward in real time using the propagator $\exp(i\hat{\mathcal{H}}t/\hbar)$ to the point x' and evaluate the eigenvalue $a(x')$ of $\hat{A}$; finally, propagate in imaginary time from x' to the original starting point x." Fig. 14.6 should be replaced by the figure shown below:



3. Page 556: For consistency with other Fourier transforms in the book, eqn. (14.6.5) should be written as

$$\tilde{C}_{AB}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}t \mathrm{e}^{-i\omega t} C_{AB}(t)$$

4. Page 558: Eqn. (14.6.14) should be supplemented with the imaginary-time mean-square displacement definition for a single particle in one dimension

$$R^2(\tau) = \langle |\hat{x}(\tau) - \hat{x}(0)|^2 \rangle$$

Eqn. (14.6.14) pertains to N particles in three dimensions. The positions operators in the equation are missing hats, and the equation should read

$$R^2(\tau) = \frac{1}{N} \sum_{i=1}^{N} \left\langle [\hat{\mathbf{r}}_i(\tau) - \hat{\mathbf{r}}_i(0)]^2 \right\rangle$$

5. Page 558: Eqn. (14.6.15) contains a small error with the placement of $\hbar$. The equation should read

$$R^2(\tau) = \frac{1}{\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega \, \frac{\mathrm{e}^{-\beta\hbar\omega/2}}{\omega^2} \tilde{C}_{vv}(\omega) \times \left\{ \cosh\left[\omega\left(\frac{\beta\hbar}{2} - \tau\right)\right] - \cosh\left(\frac{\beta\hbar\omega}{2}\right) \right\}.$$

6. Page 561: Three lines up from the bottom of the page, the "$R^2_{(\mathrm{est})}(\tau)$" should be replaced by "$\bar{R}^2(\tau)$".

7. Page 562: Factors of $\hbar$ are missing from eqn. (14.6.25). The equation should read

$$\chi^2 = \frac{1}{\beta\hbar} \int_0^{\beta\hbar} \mathrm{d}\tau \left[\frac{\bar{R}^2(\tau) - R^2(\tau)}{R^2(\tau)} \right]^2$$

Chapter 15

1. Page 571: The phrase on the last line of the page should read "Applying Hamilton's equations, these become".

2. Page 572: The "H" in eqns. (15.2.1) should be "$\mathcal{H}$", which represents the Hamiltonian in eqn. (15.2.13).

3. Page 574: The second term on the right side of eqn. (15.2.7) is incorrect. It should read

$$\frac{1}{s^2 + \omega_\alpha^2} \dot{x}_\alpha(0)$$

4. On page 577, two lines above eqn. (15.2.18), the M time points are $0, \Delta t, 2\Delta t, ..., (M-1)\Delta t$, and eqns. (15.2.18)-(15.2.20) should be defined accordingly:

$$R(k\Delta t) = \sum_{j=0}^{M-1} \left[a_k \cos\left(\frac{2\pi jk}{M}\right) + b_k \sin\left(\frac{2\pi jk}{M}\right) \right]$$

$$P(a_0, ..., a_{M-1}, b_0, ..., b_{M-1}) = \prod_{k=0}^{M-1} \frac{1}{2\pi\sigma_k^2} \, e^{-(a_k^2+b_k^2)/2\sigma_k^2}$$

$$\sigma_k^2 = \frac{kT}{M} \sum_{j=0}^{M-1} \zeta(j\Delta t) \cos\left(\frac{2\pi jk}{M}\right)$$

5. Page 590: Eqn. (15.5.11) should read:

$$v(s) \approx v(t) + (s-t)f(q(t)) - (s-t)\gamma v(t) + \sigma \left[w(s) - w(t) \right].$$

6. Page 596: Eqn. (15.7.10) should read:

$$\boldsymbol{\Omega} = \langle L\mathbf{A}\mathbf{A}^\dagger \rangle \langle \mathbf{A}\mathbf{A}^\dagger \rangle^{-1}.$$

7. On page 596, in eqn. (15.7.12), the integral is missing a factor $\exp(-st)$ needed for the Laplace transform. The equation should read

$$\int_0^\infty \mathrm{d}t \; \mathrm{e}^{-st} \left[\mathrm{e}^{iLt} - \mathrm{e}^{\mathcal{Q}iLt} \right] = (s - iL)^{-1} - (s - \mathcal{Q}iL)^{-1}.$$

Chapter 16

1. Page 631: Three lines below Fig. 16.13, replace "simple" by "single".

Appendix A

1. Page 651: On the right side of eqn. (A.16), the $\bar{y}_i$ should be replaced by $\bar{x}_i$ in the numerator, and a right bracket is missing in the denominator. The equation should read as

$$\delta(g(x)) = \sum_{i=1}^{n} \frac{\delta(x - \bar{x}_i)}{|g'(\bar{x}_i)|}.$$

Appendix B

1. Page 652: In eqn. (B.1), a left bracket in the equation is misplaced. The equation should read

$$U_{\rm nb}(\mathbf{r}_1, ..., \mathbf{r}_N) = \sum_{i>j\in{\rm nb}} \left\{ 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6} \right] + \frac{q_i q_j}{r_{ij}} \right\}.$$

2. Page 653: In eqn. (B.5), a left bracket in the middle line of the equation is misplaced. The equation should read

$$U_{\rm short}(\mathbf{r}_1, ..., \mathbf{r}_N) = \sum_{\mathbf{S}} \sum_{i>j\in{\rm nb}} \left\{ 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij,\mathbf{S}}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij,\mathbf{S}}}\right)^{6} \right] + \frac{q_i q_j {\rm erfc}(\alpha r_{ij,\mathbf{S}})}{r_{ij,\mathbf{S}}} \right\}$$

3. On page 662, eqn. (B.21) should read:

$$U_{\rm corr}(\mathbf{r}_1, ..., \mathbf{r}_N) = \sum_{i,j\in{\rm intra}} q_i q_j \chi(r_{ij}, g_{\rm max}) + \frac{\alpha}{\sqrt{\pi}} {\rm erfc}(g_{\rm max}/2\alpha) \sum_i q_i^2,$$

and $U_{\rm corr}(\mathbf{r}_1, ..., \mathbf{r}_N)$ should be *added* to $U_{\rm excl}(\mathbf{r}_1, ..., \mathbf{r}_N)$ in order to correct for the finite truncation of reciprocal space.

Appendix C

1. Pages 664 and 665: In eqns. (C.12)–(C.17), all factors of $\hat{Q}_h$ should be replaced by $\hat{Q}^h$.

Appendix D

1. Page 668: In eqns. (D.10) and (D.11), the Fourier transform definitions should be written as

$$g(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} {\rm d}\omega \; {\rm e}^{i\omega t} \hat{g}(\omega)$$

and

$$\hat{g}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{0}^{\infty} {\rm d}t \; g(t) {\rm e}^{-i\omega t}.$$