Errata for Version 2.0 of *Mathematical Methods for Molecular Science*

SUBSTANTIVE EDITS made to Version 2.0 to correct equations or clarify passages are listed below. Edits to correct misspellings and improve punctuation are not listed. The changes noted here are reflected in Version 2.3.

1. The discussion of odd and even functions in section 1.1.5 has been expanded.
2. On page 21, in the second paragraph, $\sin(2\pi x)$ should be $\cos(\theta)$ and x should be θ.
3. The series on page 33 should read
$$\cos\theta + i\sin\theta = 1 + i\theta + \frac{(i\theta)^2}{2!} + \frac{(i\theta)^3}{3!} + \frac{(i\theta)^4}{4!} + \frac{(i\theta)^5}{5!} + \dots$$
4. In Figure 2.12 on page 42, all logarithms are natural logarithms.
5. In exercise 2.17, the range of the imaginary component is $-i\pi$ to $i\pi$.
6. In exercise 3.22 on page 65, part (b) should say $dA(T,V) = -SdT - pdV$.
7. On page 72, the next to last sentence before section 4.2.3 should state that when the vectors are perpendicular $\mathbf{v}\cdot\mathbf{w} = 0$, as $v_w = w_v = 0$.
8. The discussion of the divergence and laplacian on pages 88 through 90 has been revised for clarity.
9. In Complements C_5 and D_5, the term *differential line element* has been replaced by *displacement vector* when referring to $d\mathbf{l}$.
10. In section 7.1.2, the first series should read
$$\sum_{n=0}^{\infty} u_n = u_1 + u_2 + u_3 + \dots$$
11. The integral on page 152 should read
$$\int \frac{1}{x^2}\, e^{-\frac{1}{x}}\, dx = -\int e^{-y}\, dy = e^{-y} + C = e^{-\frac{1}{x}} + C$$
12. The discussion in section 10.2.2 has been revised. The term *regime* has been replaced by *domain*. The discussion of Case #2 and the steady state approximation has been revised for clarity. These edits have impacted the equation numbering in this section.
13. In Complement C_{11}, the term *regime* has been replaced by *case*. In a number of instances, references to the it position of the oscillator have been corrected to refer to the *displacement* of the oscillator.
14. The coefficients on the right hand side of the equalities in the following equations on page 230 were corrected to be
$$\sum_{n=0}^{\infty} a_n n x^{n-1} \to \sum_{n=1}^{\infty} a_n n x^{n-1} = a_1 + 2a_2 x + 3a_3 x^2 + \dots$$
$$\sum_{n=1}^{\infty} a_n n x^{n-1} \to \sum_{n=0}^{\infty} a_{n+1}(n+1)x^n = a_1 + 2a_2 x + 3a_3 x^2 + \dots$$
15. The equation in footnote 14 on page 261 was corrected to refer to the classical wave equation which may be written $h_{tt} = v^2 h_{xx}$.
16. The equation ending section 12.3.1 on page 263 should read
$$\frac{\partial h}{\partial t}(x,0) = \sum_{n=1}^{\infty} t_n \omega_n \sin\left[\frac{n\pi}{L}x\right]$$
with the initial conditions referring to $h(x,0)$ and $h_t(x,0)$.

17. The third equation in section 12.3.2 on page 263 should read

$$\frac{\partial h}{\partial t}(x,0) = 0$$

18. The fourth equation on page 264 should read

$$\frac{\partial h}{\partial t}(x,0) = \sum_{n=1}^{\infty} t_n \omega_n \sin\left[\frac{n\pi}{L}x\right] = 0$$

19. In problem 12.2, the equation appearing in the first sentence on page 270 should read $h_{tt}(x,t) = v^2 h_{xx}(x,t)$.
20. In Chapter 12, references to *one dimension*, *one-dimensional*, *two dimension*, and *two-dimensional* have been revised for consistency.
21. The formula appearing in footnote 27 on page 291 should read

$$\frac{dk_n}{dn} = \frac{2\pi}{L}$$

22. The first equation on page 292 should read

$$\Delta k_n = \frac{2\pi}{L} \to dk$$

23. The fourth equation on page 292 should read

$$f(x) = \int_{-\infty}^{\infty} \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} f(x')\, \mathrm{e}^{-ikx'} dx'\right] \mathrm{e}^{ikx} dk = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(k) \mathrm{e}^{ikx} dk$$

24. The equation in exercise 13.11 on page 308 should read

$$f(t) = \begin{cases} \frac{2t}{T} & -\frac{T}{2} \le t < \frac{T}{2} \\ 2\left(1 - \frac{t}{T}\right) & \frac{T}{2} \le t < \frac{3T}{2} \end{cases}$$

25. The equation in problem 13.14 on page 308 should read

$$h(x) = \sin\left(\frac{\pi x}{L}\right)$$
