CORRECTIONS

Please write about typos and errors to
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page 59, Eq. (2.14)

The star on $V_{b,a}$ should be deleted. Equation should read

$V_{a,b} = Ve^{-i\eta}$; $V_{b,a} = Ve^{i\eta}$

page 64, line below Eq. (2.36)

"where each function" → "where, for non-interacting subsystems, each function"

page 64, line above Eq. (2.40a):

The following footnote should be inserted after "yields": This is a gross oversimplification. A proper derivation of Eqs. (2.40) relies on time dependent variational theory (see, e.g. A. D. McLachlan, Mol. Phys. **7**, 139 (1964))

Pages 72 and 73:

The text above Eq. (2.51) and the text below Eq. (2.52) contain the notation $\psi_{n,v}(\mathbf{r},\mathbf{R})$ for the vibronic wavefunction, while in Eq. (2.53) the same wavefunction appears as $\psi_v^{(n)}(\mathbf{r},\mathbf{R})$. These notations are equivalent.

Page 100, Eq. 2.194

On the RHS, $\Psi(t=0)$ should be replaced by $\Psi(t)$.

Page 119, line 4 of footnote 3

(1) First line of page 3.2.3:
"As an application to the results" → "As an application of the results"

(2)Please change (add text in parenthesis):
"and, the density of states used below…." →
"and (as already noted below Eq. (3.20)), the density of states used below…."

Page 123, line above Eq. (3.44)

"Eqs. (3.32d), (3.38), 3.41) and (1.29)" → "Eqs. (3.32d), (3.38), (3.39), (3.41) and (1.29)"

Page 123, Eq. (3.45)

$\frac{1}{\varepsilon}$ is missing on the RHS. The equation should be:

$$\Phi(\mathbf{r},t) = \frac{1}{\varepsilon}\int d^3r' \frac{\rho(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}$$

Page 180, 2nd line

"per unit volume → per unit square volume

Page 199, 4th line of Section 6.2.3

"except of" → "except for"

Page 207, line above Eq. (6.63)

"If $\hat{A}$ and $\hat{B}$ are real operators" → "If the Schrödinger representations $\hat{A}$ and $\hat{B}$ are real operators (in the sense that $\hat{A}^*$ is obtained from $\hat{A}$ by replacing all parameters by their complex conjugates)"

Page 214, lines 4-5 below Eq. 6.93)

(1) ("an explicit example is given in Section 8.2.5)" → ("an explicit example is given in sections 8.2.5-8.2.6)"

Page 214, 2nd line below Eq. (6.94)

"We will see in Section 8.2.5" → "We will see in Section 8.2.6"

Page 234, Eq. 7.43

Remove < > from the expression on the RHS. The expression should be:

$$C(t_2,t_1) = \lim_{N\to\infty} \frac{1}{N}\sum_{k=1}^{N} z^{(k)}(t_2) z^{(k)}(t_1)$$

Page 235, Eq. 7.44

Remove < > from the expression on the RHS. The expression should be:

$$C(t) = \lim_{N\to\infty} \frac{1}{N}\sum_{k=1}^{N} z(t_k + t) z(t_k)$$

Page 294, line above Eq. 8.151

"probability to remain in the interval" should be "probability not to remain in the interval"

page 311, line 1

"where $\Lambda_1(E)$ and $\Lambda_1(E)$ are" → "where $\Lambda_1(E)$ and $\Gamma_1(E)$ are"

page 369, line 1

"Using the definitions (10.63a) and (10.58) show that" → "Using the definitions (10.63a), (10.64) and (10.58) show that"

page 373, line after Eq. (10.109)

"5 and formally integrate it to get" → "and formally integrate it to get" (eliminate "5")

page 377, line above Eq. (10.127)

"the more general case (10.22) is" → "the more general case (10.122) is"

page 378, second line of problem 10.18

"the more general case (10.113) is" → "the more general case (10.122) is"

page 388, next to last line in the second paragraph.

Insert space after $\tilde{C}(0)$

Page 401, Eq. 11.6

The last term on the RHS: Instead of $O\left[(\beta\Delta H)^2\right]$ should be $O\left[(\beta H_1)^2\right]$

Page 403, Eq. (11.17)

In the middle term, $\int d\mathbf{r}^N \int d\mathbf{r}^N$ should be replaced by $\int d\mathbf{r}^N \int d\mathbf{p}^N$. Also, H_0 should be replaced by $\hat{H}_0$. The full equation should be

$$f\left(\mathbf{r}^N, \mathbf{p}^N; -\infty\right) = \frac{e^{-\beta \hat{H}_0}}{\int d\mathbf{r}^N \int \mathbf{p}^N e^{-\beta \hat{H}_0}} \; ; \quad \hat{\rho}(-\infty) = \frac{e^{-\beta \hat{H}_0}}{Tr\left[e^{-\beta \hat{H}_0}\right]}$$

Page 404, Eq. (11.21)

In the integrand on the right, $\chi_{AB}(t)$ should be replaced by $\chi_{BA}(t)$. The full expression should be

$$\beta\langle\delta A(0)\delta B(t)\rangle_0 = \int_{-\infty}^{0} dt' \chi_{BA}(t-t') = \int_{t}^{\infty} d\tau \chi_{BA}(\tau)$$

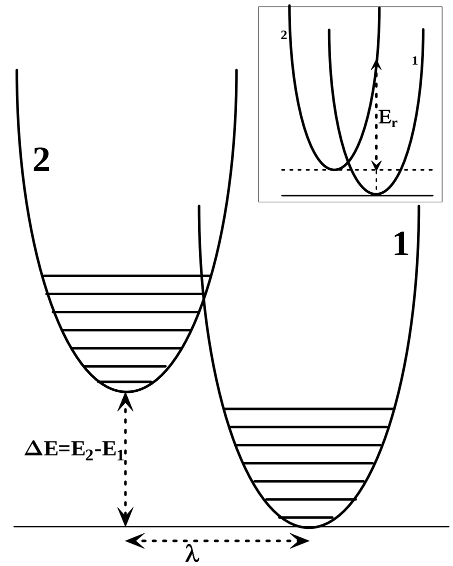
Page 408, line following Eq. (11.42)

"Using integral" → Using an integral"

Page 428, in the little box of Fig. 12.3

(Correction contributed by Fox Zeng <fox.tseng@gmail.com>)

The double sided arrow denoting the reorganization energy is wrong. The correct Figure 12.3 is:



page 431, line 12 from bottom (3rd line in the paragraph that starts with "(b) The couplings")

(2.28) → (12.28) and (2.29) → (12.28)

page 436, Last line

"Heisenberg representation (with respect to $\hat{H}_B$) operator" → "Heisenberg representation (with respect to $\hat{H}_B$) operator"

page 438, line below Eq. 12.52

"(for an operator $\hat{A}$ that is…)" → "(for harmonic oscillator Hamiltonian and an operator $\hat{A}$ that is…)"

page 445, line 7

"are the $n_c!/\bar{v}!$ terms with $v_\alpha = 1$ or 0, so that $k_{1\leftarrow 2}(\omega_{21}) \sim \bar{\lambda}^{2\bar{v}} n_c!/\bar{v}!$ is essentially the same as (12.64) and…" →
"are the $n_c!/\left(\bar{v}!(n_c - \bar{v})!\right)$ terms with $v_\alpha = 1$ or 0, so that
$k_{1\leftarrow 2}(\omega_{21}) \sim \bar{\lambda}^{2\bar{v}} n_c!/\left(\bar{v}!(n_c - \bar{v})!\right)$ is the analog of (12.64) and…"

Page 445, 4th line of Section 12.5.4

(Following question by Sangkook Choi sangkookchoi@gmail.com)

Add a footnote after "factors."(This should be footnote 9, the following footnotes in Chapter 12 will need to be renumbered in the footnote list and in the text)

NEW FOOTNOTE 9: Applying the short time approximation should be done with care. The physics has to be such that the correlation function remains zero (or at least unimportant) after it became zero at short time. The result does not depend on what is the physical process (e.g., broadening by the surrounding liquid) that makes this happen.

page 563, 3rd line in 2nd paragraph.

"that is same" → "that is, same" or "that is the same"

page 564, second line of Eq. (16.25)

(Correction contributed by Akihito Ishizaki <ishizaki@kuchem.kyoto-u.ac.jp>)

The phrase "*text*(*but not*" should be replaced by "(but not"

page 572, first paragraph.

added commas enlarged in red

It is important to realize that the only approximations that enter into this rate expression is the use of the Fermi golden-rule, which is compatible with the weak coupling non-adiabatic limit, and the Condon approximation, which is known to be successful in applications to electronic spectroscopy. The solvent effect on the electronic process, including the slow dielectric response, must arise from the FC factor that contains contributions from all the surrounding intermolecular and intramolecular nuclear degrees of freedom. In fact, if the nuclear component of the solvent polarization was the only important nuclear motion in the system, then Eqs. (16.53) and (16.51) should be equivalent. This implies that in this case

page 573 first paragraph (lines 4-5 from top)

The terms "inner shell" and "outer shell" should be replaced by by the more common "inner sphere" and "outer sphere" as used in other places in chapter 16.

page 575, Eqs. 16.68-16.70 should change according to (changes in red)

$$F_{ba} = C_{ab}\exp\left(-\beta\frac{\left(\Delta E - E_r^{(ab)}\right)^2}{4E_r^{(ab)}}\right);\quad F_{ab} = C_{ab}\exp\left(-\beta\frac{\left(\Delta E + E_r^{(ab)}\right)^2}{4E_r^{(ab)}}\right) \qquad (16.68a)$$

$$F_{ii} = C_{ii}\exp\left(-\beta\frac{E_r^{(ii)}}{4}\right);\qquad i = a,b \qquad (16.68b)$$

$$\frac{k_{ba}}{\left(k_{aa}k_{bb}\right)^{1/2}} = \frac{F_{ba}}{\left(F_{aa}F_{bb}\right)^{1/2}} = \frac{C_{ab}}{\sqrt{C_{aa}C_{bb}}}\exp\left[-\beta\left(\frac{\left(\Delta E - \left(E_r^{(aa)} + E_r^{(bb)}\right)/2\right)^2}{2\left(E_r^{(aa)} + E_r^{(bb)}\right)} + \frac{E_r^{(aa)}}{8} + \frac{E_r^{(bb)}}{8}\right)\right]$$

$$= \frac{C_{ab}}{\sqrt{C_{aa}C_{bb}}}\exp\left(-\beta\frac{\Delta E^2}{2\left(E_r^{(aa)} + E_r^{(bb)}\right)}\right)\exp\left(+\beta\Delta E/2\right)$$

(16.69)

$$k_{ba} = \left(\frac{k_{aa} k_{bb} K}{C_{aa} C_{bb}} \right)^{1/2} C_{ab} \exp\left(-\beta \frac{\Delta E^2}{2\left(E_r^{(aa)} + E_r^{(bb)} \right)} \right) \tag{16.70}$$

<u>Page 587, line above (16.90)</u>

"…with the corresponding charge distribution" → "…with the charge distribution $P_n^{(l)}(\mathbf{r})$"

<u>Page 634, Eq. (17.42)</u>

In the expression on the right, 0 should be replaced by $N+1$ in 4 places. The equation should read:

$$\hat{H}_{SL} = \sum_l \left(H_{0,l} |0\rangle\langle l| + H_{l,0} |l\rangle\langle 0| \right); \qquad \hat{H}_{SR} = \sum_r \left(H_{N+1,r} |N+1\rangle\langle r| + H_{r,N+1} |r\rangle\langle N+1| \right)$$

<u>Page 644, two last lines</u>

problem --> problems

<u>Page 652, 8 lines from bottom</u>

"out" → our

<u>Page 653, 5 lines above Eq. (18.21)</u>

"out" ---> "|out>"

<u>Page 706, Eq. (18.136)</u>

In the numerator, the last term in parentheses is missing an E: "$_{in,out}$" should be "$E_{in,out}$". The full equation should be

$$\operatorname{Im}\left(\frac{1}{\left(E_{in,s} + (1/2)i\gamma_s\right)\left(E_{out,s} - (1/2)i\gamma_s\right)\left(E_{in,out} + (1/2)i\eta\right)} \right)$$
$$= \frac{\operatorname{Im}\left[\left(E_{in,s} - (1/2)i\gamma_s\right)\left(E_{out,s} + (1/2)i\gamma_s\right)\left(E_{in,out} - (1/2)i\eta\right) \right]}{\left(E_{in,s}{}^2 + ((1/2)\gamma_s)^2\right)\left(E_{out,s}{}^2 + ((1/2)\gamma_s)^2\right)\left(E_{in,out}{}^2 + ((1/2)\eta)^2\right)}$$

Special thanks to Michael Galperin and Joe Subotnik for pointing out many corrections

(last updated May 21, 2013)