CORRECTIONS

V. May and O. Kühn

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REPLACE:

$$\Theta_{ab} = \int dr\ \phi_a(r;R)\, T_{\mathrm{nuc}}\, \phi_b(r;R) + \sum_n \frac{1}{M_n} \left[\int dr\ \phi_a(r;R)\mathbf{P}_n \phi_b(r;R) \right] \mathbf{P}_n \tag{2.17}$$

BY:

$$\Theta_{ab} = \int dr\ \phi_a^*(r;R)\, T_{\mathrm{nuc}}\, \phi_b(r;R) + \sum_n \frac{1}{M_n} \left[\int dr\ \phi_a^*(r;R)\mathbf{P}_n \phi_b(r;R) \right] \mathbf{P}_n \tag{2.17}$$

REPLACE:

$$\langle \chi_{aM} | \chi_{bN} \rangle = \sqrt{\frac{N-1}{N}} \frac{c2-\epsilon}{1+\epsilon} \langle \chi_{aM} | \chi_{bN-1} \rangle - \frac{2g\sqrt{\epsilon}}{\sqrt{N}(1+\epsilon)} \langle \chi_{aM} | \chi_{bN-1} \rangle + \sqrt{\frac{M\epsilon}{N}} \frac{2}{1+\epsilon} \langle \chi_{aM-1} | \chi_{bN-1} \rangle \tag{2.147}$$

and

$$\langle \chi_{aM} | \chi_{bN} \rangle = -\sqrt{\frac{M-1}{M}} \frac{c2-\epsilon}{1+\epsilon} \langle \chi_{aM-2} | \chi_{bN} \rangle + \frac{2g}{\sqrt{M}(1+\epsilon)} \langle \chi_{aM-1} | \chi_{bN} \rangle + \sqrt{\frac{N\epsilon}{M}} \frac{2}{1+\epsilon} \langle \chi_{aM-1} | \chi_{bN-1} \rangle \tag{2.148}$$

BY:

$$\langle \chi_{aM} | \chi_{bN} \rangle = \sqrt{\frac{N-1}{N}} \frac{1-\epsilon}{1+\epsilon} \langle \chi_{aM} | \chi_{bN-2} \rangle - \frac{2g\sqrt{\epsilon}}{\sqrt{N}(1+\epsilon)} \langle \chi_{aM} | \chi_{bN-1} \rangle + \sqrt{\frac{M\epsilon}{N}} \frac{2}{1+\epsilon} \langle \chi_{aM-1} | \chi_{bN-1} \rangle \tag{2.147}$$

and

$$\langle \chi_{aM} | \chi_{bN} \rangle = -\sqrt{\frac{M-1}{M}} \frac{1-\epsilon}{1+\epsilon} \langle \chi_{aM-2} | \chi_{bN} \rangle + \frac{2g}{\sqrt{M}(1+\epsilon)} \langle \chi_{aM-1} | \chi_{bN} \rangle + \sqrt{\frac{N\epsilon}{M}} \frac{2}{1+\epsilon} \langle \chi_{aM-1} | \chi_{bN-1} \rangle \tag{2.148}$$

REPLACE:

$$\rho(s,\bar{s}) = \int dZ\,\Psi^*(s,Z)\Psi(\bar{s},Z) \tag{3.6}$$

BY:

$$\rho(s,\bar{s}) = \int dZ\,\Psi(s,Z)\Psi^*(\bar{s},Z) \tag{3.6}$$

REPLACE:

$$\langle\hat{O}\rangle = \int ds\,[O(\bar{s})\rho(s,\bar{s})]_{s=\bar{s}} \tag{3.7}$$

BY:

$$\langle\hat{O}\rangle = \int ds\,[O(s)\rho(s,\bar{s})]_{s=\bar{s}} \tag{3.7}$$

REPLACE:

$$\rho(s,\bar{s}) = \Phi_{\mathrm{S}}^*(s)\Phi_{\mathrm{S}}(\bar{s}) \tag{3.8}$$

BY:

$$\rho(s,\bar{s}) = \Phi_{\mathrm{S}}(s)\Phi_{\mathrm{S}}^*(\bar{s}) \tag{3.8}$$

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REPLACE:

$$\frac{\partial}{\partial t} E_{\mathrm{S}} = \mathrm{tr}_{\mathrm{S}}\{H_{\mathrm{S}} \mathcal{D} \hat{\rho}(t)\} = \sum_u \mathrm{tr}_{\mathrm{S}}\{[H_{\mathrm{S}}, K_u]_-(\Lambda_u \hat{\rho}(t) - \hat{\rho}(t)\Lambda_u^{(+)})\} \tag{3.267}$$

BY:

$$\frac{\partial}{\partial t} E_{\mathrm{S}} = -\mathrm{tr}_{\mathrm{S}}\{H_{\mathrm{S}} \mathcal{D} \hat{\rho}(t)\} = -\sum_u \mathrm{tr}_{\mathrm{S}}\{[H_{\mathrm{S}}, K_u]_-(\Lambda_u \hat{\rho}(t) - \hat{\rho}(t)\Lambda_u^{(+)})\} \tag{3.267}$$

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REPLACE:

$$\begin{aligned} \left(\frac{\partial \hat{\rho}(t)}{\partial t}\right)_{\mathrm{diss}} &= -\sum_{a,b} \left\{ \frac{1}{2} \Big[k_{ab} |a\rangle\langle a|, \hat{\rho}(t) \Big]_+ - k_{ab} |b\rangle\langle a|\hat{\rho}(t)|a\rangle\langle b| \right\} \\ &\quad + \sum_{a,b} \gamma_{ab}^{(\mathrm{pd})} |a\rangle\langle a|\hat{\rho}(t)|b\rangle\langle b| \end{aligned} \tag{3.307}$$

BY:

$$\begin{aligned} \left(\frac{\partial \hat{\rho}(t)}{\partial t}\right)_{\mathrm{diss}} &= -\sum_{a,b} \left\{ \frac{1}{2} \Big[k_{ab} |a\rangle\langle a|, \hat{\rho}(t) \Big]_+ - k_{ab} |b\rangle\langle a|\hat{\rho}(t)|a\rangle\langle b| \right\} \\ &\quad - \sum_{a,b} \gamma_{ab}^{(\mathrm{pd})} |a\rangle\langle a|\hat{\rho}(t)|b\rangle\langle b| \end{aligned} \tag{3.307}$$

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REPLACE:

$$\begin{aligned} \frac{\partial}{\partial t}\hat{\rho}(Z,\bar{Z};t) &= -\frac{i}{\hbar}\left(H_{\mathrm{S}} + H_{\mathrm{S-R}}(Z) + H_{\mathrm{R}}(Z)\right)\hat{\rho}(Z,\bar{Z};t) \\ &\quad -\hat{\rho}(Z,\bar{Z};t)\Big(H_{\mathrm{S}} + H_{\mathrm{S-R}}(Z) + H_{\mathrm{R}}(\bar{Z}\Big) \end{aligned} \tag{3.423}$$

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REPLACE:

$$C_{\mathrm{d-d}}(t) =| d_{eg} e^{-i\omega_{eg}} |^2 \langle S_{eg}(t,0)\rangle_g =| d_{eg} |^2 e^{-i\omega_{eg}-\Gamma(t)} \tag{5.580}$$

BY:

$$C_{\mathrm{d-d}}(t) = | d_{eg} |^2 e^{-i\omega_{eg}t} \langle S_{eg}(t,0)\rangle_g = | d_{eg} |^2 e^{-i\omega_{eg}t-\Gamma(t)} \tag{5.580}$$

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REPLACE:

$$i\hbar \frac{\partial}{\partial t}\mathbf{r}_j = [\mathbf{r}_j, H_{\mathrm{el}}]_- = \frac{\mathbf{p}_j}{m_{\mathrm{el}}} \tag{5.104}$$

and *BY:*

$$i\hbar \frac{\partial}{\partial t}\mathbf{r}_j = [\mathbf{r}_j, H_{\mathrm{el}}]_- = i\hbar \frac{\mathbf{p}_j}{m_{\mathrm{el}}} \tag{5.104}$$

REPLACE:

$$\begin{aligned}\langle\phi_e|\sum_j \mathbf{e}_\lambda \mathbf{p}_j|\phi_g\rangle &= m_{\rm el}\mathbf{n}_\lambda \sum_j \langle\phi_e\,|(\mathbf{r}_j H_{\rm el} - H_{\rm el}\,\mathbf{r}_j)|\,\phi_g\rangle \\ &= m_{\rm el}\mathbf{n}_\lambda (E_g - E_e)\sum_j \langle\phi_e\,|\mathbf{r}_j|\,\phi_g\rangle \\ &= -\frac{m_{\rm el}}{e}(E_e - E_g)\mathbf{n}_\lambda \mathbf{d}_{eg} \qquad (5.105)\end{aligned}$$

and

$$I(\omega) = \frac{4\hbar\omega^3}{3c^3}|\mathbf{d}_{eg}|^2 \sum_{M,N} f(E_{eM})|\langle\chi_{eM}|\chi_{gN}\rangle|^2 \delta(E_{eM} - E_{gN} - \hbar\omega) \qquad (5.107)$$

and

$$I(\omega) = \frac{4\hbar\omega^3}{3c^3}|\mathbf{d}_{eg}|^2 \mathcal{D}_{\rm em}(\omega - \omega_{eg}) \qquad (5.108)$$

BY:

$$\begin{aligned}\langle\phi_e|\sum_j \mathbf{e}_\lambda \mathbf{p}_j|\phi_g\rangle &= \frac{m_{\rm el}}{i\hbar}\mathbf{n}_\lambda \sum_j \langle\phi_e\,|(\mathbf{r}_j H_{\rm el} - H_{\rm el}\,\mathbf{r}_j)|\,\phi_g\rangle \\ &= \frac{m_{\rm el}}{i\hbar}\mathbf{n}_\lambda (E_g - E_e)\sum_j \langle\phi_e\,|\mathbf{r}_j|\,\phi_g\rangle \\ &= -\frac{m_{\rm el}}{i\hbar e}(E_e - E_g)\mathbf{n}_\lambda \mathbf{d}_{eg} \qquad (5.105)\end{aligned}$$

and

$$I(\omega) = \frac{4\omega^3}{3c^3}|\mathbf{d}_{eg}|^2 \sum_{M,N} f(E_{eM})|\langle\chi_{eM}|\chi_{gN}\rangle|^2 \delta(E_{eM} - E_{gN} - \hbar\omega) \qquad (5.107)$$

and

$$I(\omega) = \frac{4\omega^3}{3c^3}|\mathbf{d}_{eg}|^2 \mathcal{D}_{\rm em}(\omega - \omega_{eg}) \qquad (5.108)$$

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REPLACE:

Here, the reference driving force $\Delta E \equiv E_{D0} - E_{A0}$ has been introduced; its actual value is reduced by $\hbar\omega_{\rm intra}N$. Often Eq. (6.106) for the ET rate is written using a more explicit expression for the Franck–Condon factor $|\langle\chi_{D0}|\chi_{AN}\rangle|^2$. Making use of the derivations given in Section 2.98 and replacing the shift $g_{\rm intra}$ of the PES of the intramolecular vibration by

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REPLACE:

$$\begin{aligned} J_{mn}(ab,cd) &\equiv \langle\varphi_{ma}\varphi_{nb}|V_{mn}|\varphi_{nc}\varphi_{md}\rangle \\ &= \int dr_m dr_n\; \varphi^*_{ma}(r_m)\varphi^*_{nb}(r_n)V^{(\rm el-el)}_{mn}(r_m,r_n)\varphi_{nc}(r_n)\varphi_{md}(r_m) \\ &+ \delta_{ad}\delta_{bc}V^{(\rm nuc-nuc)}_{mn} \\ &+ \delta_{bc}\int dr_m\varphi^*_{ma}(r_m)V^{(\rm el-nuc)}_{mn}(r_m,R^{(\rm intra)}_n)\varphi_{md}(r_m) \\ &+ \delta_{bc}\int dr_n\varphi^*_{nb}(r_n)V^{(\rm nuc-el)}_{mn}(R^{(\rm intra)}_m,r_n)\varphi_{nc}(r_n) \end{aligned} \tag{8.10}$$

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$$\begin{aligned} J_{mn}(ab,cd) &\equiv \langle\varphi_{ma}\varphi_{nb}|V_{mn}|\varphi_{nc}\varphi_{md}\rangle \\ &= \int dr_m dr_n\; \varphi^*_{ma}(r_m)\varphi^*_{nb}(r_n)V^{(\rm el-el)}_{mn}(r_m,r_n)\varphi_{nc}(r_n)\varphi_{md}(r_m) \\ &+ \delta_{ad}\delta_{bc}V^{(\rm nuc-nuc)}_{mn} \\ &+ \delta_{bc}\int dr_m\varphi^*_{ma}(r_m)V^{(\rm el-nuc)}_{mn}(r_m,R^{(\rm intra)}_n)\varphi_{md}(r_m) \\ &+ \delta_{ad}\int dr_n\varphi^*_{nb}(r_n)V^{(\rm nuc-el)}_{mn}(R^{(\rm intra)}_m,r_n)\varphi_{nc}(r_n) \end{aligned} \tag{8.10}$$

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REPLACE:

$$\sum_{\{a\}} = |\phi^{\mathrm{HP}}_{\{a\}}\rangle\langle\phi^{\mathrm{HP}}_{\{a\}}| = |0\rangle\langle 0| + \sum_m |m\rangle\langle m| + \sum_{m,n} |mn\rangle\langle mn| + \dots \tag{8.32}$$

BY:

$$\sum_{\{a\}} |\phi^{\mathrm{HP}}_{\{a\}}\rangle\langle\phi^{\mathrm{HP}}_{\{a\}}| = |0\rangle\langle 0| + \sum_m |m\rangle\langle m| + \sum_{m,n} |mn\rangle\langle mn| + \dots \tag{8.32}$$

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REPLACE:

$$U_\alpha(q) = \mathcal{E}_\alpha - \sum_\xi \hbar\omega_\xi g^2_{\alpha\alpha}(\xi) + \sum_\xi \frac{\hbar\omega_\xi}{4}\Big(Q_\xi + 2g_{\alpha\alpha}(\xi)\Big) \tag{8.79}$$

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REPLACE:

Figure 8.11: Dissipative dynamics in a regular chain of seven molecules: (a) transition amplitudes at the corresponding single–exciton eigenenergies, (b) relaxation matrix $w_{1\alpha}$ for $g_{mn} = 0.77J$ and $\hbar\omega_c = 0.25J$ (black T=300 K, grey T=4 K). Panels (c) and (d): $\rho_{\alpha\alpha}(t) = P_\alpha(t)$ for T=300 K (c) and T=4 K (d).

BY:

Figure 8.11: Dissipative dynamics in a regular chain of seven molecules: (a) transition amplitudes at the corresponding single–exciton eigenenergies, (b) relaxation matrix $k_{1\alpha}$ for $g_{mn} = 0.77J$ and $\hbar\omega_c = 0.25J$ (black T=300 K, grey T=4 K). Panels (c) and (d): $\rho_{\alpha\alpha}(t) = P_\alpha(t)$ for T=300 K (c) and T=4 K (d).

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REPLACE:

This expression confirms the principal existence of some $\tilde{\mathcal{U}}$ in Eq. (9.24). Given the form Eq. (9.32) for $\mathcal{U}$ one can obtain $\mathcal{U}^+$ or equivalently the equations of motion for $\hat{\sigma}$. To do this we use Eq. (9.16) and get

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