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ERRATUM

Chemomechanical Coupling of Molecular Motors: Thermodynamics, Network Representations, and Balance Conditions

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The derivation of (6.15) contains an implicit assumption that restricts its general validity and led to a wrong conclusion about the two relations (9.3) and (9.4).

As explained in Sect. 4.1, each motor state i corresponds to an ensemble of substates, which is characterized by the Helmholtz free energy H_i and the internal energy U_i, see (4.2) and (4.3). These two quantities define the entropy $S_i = (U_i - H_i)/T$ of state i at temperature T. During a transition $|ij\rangle$ from state i to state j, the motor produces, on average, the entropy $\Delta S_{ij} = k_B \ln(\omega_{ij}/\omega_{ji})$, see (6.13). We then identified $T\Delta S_{ij}$ with the average heat Q_{ij} that the motor releases during the transition $|ij\rangle$ into the heat reservoir. The latter identification is, however, restricted to motor states i and j with $S_i = S_j$.

For the more general case with $S_i \neq S_j$, the average produced entropy during the transition $|ij\rangle$ satisfies the relation

$$\Delta S_{ij} = k_B \ln(\omega_{ij}/\omega_{ji}) = S_j - S_i + Q_{ij}/T \tag{1}$$

where $S_j - S_i$ and Q_{ij}/T represent the entropy change of the motor molecule and of the heat bath, respectively. The entropy differences $S_j - S_i$ cancel out from the entropies $\Delta S(\mathcal{C}^d_\nu)$ for the dicycles $\mathcal{C}^d_\nu$, see (6.8), as well as from the entropy production rates (6.7) and (6.6). Indeed, the general expression (6.6) for the entropy production rate in the steady state remains unchanged if we substitute $\ln(\omega_{ij}/\omega_{ji})$ by $\ln(\omega_{ij}/\omega_{ji}) + A_j - A_i$ with any state function A_i as follows from flux conservation at each state (or vertex) i. Therefore, the decomposition (1) is not directly imposed by the form of (6.6) but is consistent with the corresponding

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decomposition of macroscopic systems [1] and can be checked directly for a system consisting of only two states i and j not coupled to any other reservoir apart from the heat bath.

When the relation (1) is inserted into the local energy balance relation (4.4), one obtains the free energy differences

$$H_j - H_i = U_j - U_i - T(S_j - S_i) = \Delta\mu_{ij} - \ell_{ij} F - k_B T \ln(\omega_{ij}/\omega_{ji}), \tag{2}$$

which generalizes (6.15) to the case $S_i \neq S_j$.

All relations of our article that follow after equation (6.15) and involve the internal energies can now be generalized by simply replacing the internal energies U_i by the free energies H_i. When this substitution is made in equations (8.1)–(8.4), for example, one obtains explicit expressions for the landscape of the free energies H_i. Likewise, the constrained equilibrium relation (9.3) now attains the more general form

$$\frac{\omega_{ba}}{\omega_{ab}} = \frac{\exp[-H_a/k_B T]}{\exp[-H_b/k_B T]} e^{(-\Delta\mu_{ab}+\ell_{ab}F)/k_B T} \equiv \frac{P_a^{\mathrm{ce}}}{P_b^{\mathrm{ce}}}. \tag{3}$$

For $F = 0$, i.e., in the absence of a work reservoir, (3) reduces to relation (9.4) as obtained by Hill and Simmons [2].

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References

1. Callen, H.B.: Thermodynamics and an Introduction to Thermostatistics. Wiley, New York (1985)
2. Hill, T.L., Simmons, R.M.: Free energy levels and entropy production associated with biochemical kinetic diagrams. Proc. Nat. Acad. Sci. U.S.A. **73**, 95–99 (1976)