A4.2. Detailed Balance

Consider the problem of finding $\mathbf{\Pi}$ whose stationary state is a known equilibrium distribution $P(a)$.

We assume Γ is connected so that

$$P(a) > 0 \qquad \forall\ a \in \Gamma \qquad \text{(a)}$$

The search is simplified if we impose the detailed balance condition

$$\Pi_{ab}\, P(b) = \Pi_{ba}\, P(a) \qquad \forall\ a,\ b \in \Gamma \qquad \text{(A4.10)}$$

or

$$\mathbf{\Pi}\, \mathbf{D} = \mathbf{D}\, \mathbf{\Pi}^T \qquad \text{(A4.10m)}$$

where

$$\mathbf{D} = \{\, \delta_{ab}\, P(a) \,\} = \text{diag}[\, \{\, P(1),\ \ldots,\ P(N) \,\}\,]$$

Note that with $\mathbf{U} = (1,\ \ldots,\ 1)^T$,

$$\mathbf{U}^T\, \mathbf{D} = \mathbf{P}^T \qquad \& \qquad \mathbf{D}\, \mathbf{U} = \mathbf{P}$$

Eq(A4.10a) thus becomes

$$\sum_c \Pi_{ac}\, D_{cb} = \sum_c D_{ac}\, \Pi_{bc}$$

$$\rightarrow \qquad \sum_c \Pi_{ac}\, \delta_{cb}\, P(b) = \sum_c \delta_{ac}\, P(a)\, \Pi_{bc}$$

or $\quad \Pi_{ab}\, P(b) = \Pi_{ba}\, P(a) \qquad$ as expected

Eq(A4.10) implies

$$\sum_b \Pi_{ab}\, P(b) = \sum_b \Pi_{ba}\, P(a)$$

$$= P(a) \qquad [\text{ Eq(A4.1) used }]$$

In matrix form, the above becomes

$$\mathbf{\Pi}\, \mathbf{D}\, \mathbf{U} = \mathbf{D}\, \mathbf{\Pi}^T\, \mathbf{U}$$

$$\rightarrow \qquad \mathbf{\Pi}\, \mathbf{P} = \left(\mathbf{U}^T\, \mathbf{\Pi}\, \mathbf{D}\right)^T = \left(\mathbf{U}^T\, \mathbf{D}\right)^T = \mathbf{P} \qquad [\ \mathbf{U}^T\, \mathbf{\Pi} = \mathbf{U}^T \text{ used }]$$

which means $\mathbf{P}$ is a equilibrium distribution.

By re-tracing the foregoing argument, one can show that the detailed balance is the necessary & sufficient condition for equilibrium.

The advantage of switching to the detailed balance condition is that we can switch to an equivalent symmetric transfer matrix $\tilde{\mathbf{\Pi}}$ as follows. By eq(a), we can set

$$\tilde{P}_n(a) = \frac{P_n(a)}{\sqrt{P(a)}} \qquad \text{(A4.12)}$$

or $\quad \tilde{\mathbf{P}}_n = \mathbf{D}^{-1/2}\, \mathbf{P}_n \qquad$ (A4.12m)

The evolution eq(A4.2) then becomes

$$\tilde{P}_{n+1}(a) = \sum_b \sqrt{\frac{P(b)}{P(a)}}\ \Pi_{ab}\, \tilde{P}_n(a)$$

$$= \sum_b \tilde{\Pi}_{ab}\, \tilde{P}_n(a) \qquad \text{(A4.13)}$$

where

$$\tilde{\Pi}_{ab} = \sqrt{\frac{P(b)}{P(a)}}\ \Pi_{ab} \qquad \text{(A4.14)}$$

or, in matrix form

$\boldsymbol{P}_{n+1} = \boldsymbol{\Pi}\, \boldsymbol{P}_n$

→ $\tilde{\boldsymbol{P}}_{n+1} = \boldsymbol{D}^{-1/2}\, \boldsymbol{\Pi}\, \boldsymbol{D}^{1/2}\, \tilde{\boldsymbol{P}}_n$

∴ $\tilde{\boldsymbol{P}}_{n+1} = \tilde{\boldsymbol{\Pi}}\, \tilde{\boldsymbol{P}}_n$ (A4.13m)

where

$\tilde{\boldsymbol{\Pi}} = \boldsymbol{D}^{-1/2}\, \boldsymbol{\Pi}\, \boldsymbol{D}^{1/2}$ (A4.14m)

Checking for consistency, we have

$$\tilde{\Pi}_{a b} = \sum_{c d} D_{a c}^{-1/2}\, \Pi_{c d}\, D_{d b}^{1/2}$$

$$= \sum_{c d} \frac{1}{\sqrt{P(a)}}\, \delta_{a c}\, \Pi_{c d} \sqrt{P(b)}\, \delta_{d b}$$

$$= \sqrt{\frac{P(b)}{P(a)}}\, \Pi_{a b} \qquad \text{as expected}$$

With $a \leftrightarrow b$, we have

$$\tilde{\Pi}_{b a} = \sqrt{\frac{P(a)}{P(b)}}\, \Pi_{a b}$$

$$= \sqrt{\frac{P(b)}{P(a)}}\, \Pi_{b a} \qquad \text{[Eq(A4.10) used]}$$

$$= \tilde{\Pi}_{a b} \qquad \text{[Eq(A4.14) used]}$$

i.e., $\tilde{\boldsymbol{\Pi}}$ is symmetric.

In matrix form,

$\tilde{\boldsymbol{\Pi}}^T = \boldsymbol{D}^{1/2}\, \boldsymbol{\Pi}^T\, \boldsymbol{D}^{-1/2}$

Using

$\boldsymbol{\Pi}\, \boldsymbol{D} = \boldsymbol{D}\, \boldsymbol{\Pi}^T$ [See eq(A4.10a)]

we have

$\boldsymbol{D}^{-1/2}\, \boldsymbol{\Pi}\, \boldsymbol{D}^{1/2} = \boldsymbol{D}^{1/2}\, \boldsymbol{\Pi}^T\, \boldsymbol{D}^{-1/2}$

→ $\tilde{\boldsymbol{\Pi}}^T = \boldsymbol{D}^{-1/2}\, \boldsymbol{\Pi}\, \boldsymbol{D}^{1/2} = \tilde{\boldsymbol{\Pi}}$

Hence, the spectrum (or set of eigenvalues) of $\tilde{\boldsymbol{\Pi}}$ is real, while the respective left- & right- eigenvectors are identical. Since $\tilde{\boldsymbol{\Pi}}$ & $\boldsymbol{\Pi}$ are related by a similarity transform, they share the same eigenvalues.

Let $\nu = \pm 1$ be the only eigenvalues of $|\,\nu\,| = 1$. Then, according to §A4.1, $\tilde{\boldsymbol{\Pi}}$ takes the form

$$\tilde{\boldsymbol{\Pi}} = \begin{pmatrix} 0 & \tilde{\boldsymbol{\pi}} \\ \tilde{\boldsymbol{\pi}}^T & 0 \end{pmatrix}$$

so that the eigen-equations become

$$\tilde{\boldsymbol{\Pi}}\, \tilde{\boldsymbol{P}}^{(\pm)} = \pm\, \tilde{\boldsymbol{P}}^{(\pm)}$$

For a 2×2 matrix $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ with $\nu = \pm 1$, the corresponding eigenvectors are simply $\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$.

We therefore try the solutions

$$\tilde{\boldsymbol{P}}^{(\pm)} = \begin{pmatrix} \tilde{\boldsymbol{P}}_{+}^{(\pm)} \\ \tilde{\boldsymbol{P}}_{-}^{(\pm)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{u} \\ \pm \boldsymbol{v} \end{pmatrix} \qquad \text{(b)}$$

where the subscripts + & − denotes the components of phases +1 & $e^{i\pi} = -1$, respectively.

The eigen-equations thus become

$$\begin{pmatrix} 0 & \tilde{\boldsymbol{\pi}} \\ \tilde{\boldsymbol{\pi}}^T & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{u} \\ \pm \boldsymbol{v} \end{pmatrix} = \begin{pmatrix} \pm \tilde{\boldsymbol{\pi}} \boldsymbol{v} \\ \tilde{\boldsymbol{\pi}}^T \boldsymbol{u} \end{pmatrix} = \pm \begin{pmatrix} \boldsymbol{u} \\ \pm \boldsymbol{v} \end{pmatrix}$$

$$\rightarrow \qquad \tilde{\boldsymbol{\pi}} \boldsymbol{v} = \boldsymbol{u} \qquad \tilde{\boldsymbol{\pi}}^T \boldsymbol{u} = \boldsymbol{v} \qquad \text{(c)}$$

$$\therefore \qquad \tilde{\boldsymbol{\pi}}^{\boldsymbol{T}} \boldsymbol{u} = \tilde{\boldsymbol{\pi}}^T \tilde{\boldsymbol{\pi}} \boldsymbol{v} = \boldsymbol{v} \qquad \rightarrow \qquad \tilde{\boldsymbol{\pi}}^T \tilde{\boldsymbol{\pi}} = \boldsymbol{I}$$

$$\tilde{\boldsymbol{\pi}} \boldsymbol{v} = \tilde{\boldsymbol{\pi}} \tilde{\boldsymbol{\pi}}^T \boldsymbol{u} = \boldsymbol{u} \qquad \rightarrow \qquad \tilde{\boldsymbol{\pi}} \tilde{\boldsymbol{\pi}}^T = \boldsymbol{I}$$

i.e., $\tilde{\boldsymbol{\pi}}$ is an orthogonal matrix.

Hence,

$$\tilde{\boldsymbol{P}}_{+}^{(\pm)T} \tilde{\boldsymbol{P}}_{+}^{(\pm)} = \boldsymbol{u}^T \boldsymbol{u} = \boldsymbol{v}^T \tilde{\boldsymbol{\pi}}^T \tilde{\boldsymbol{\pi}} \boldsymbol{v} \qquad \text{[Eq(c) used]}$$

$$= \boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{v}$$

$$= \tilde{\boldsymbol{P}}_{-}^{(\pm)T} \tilde{\boldsymbol{P}}_{-}^{(\pm)}$$

which, in component form, can be written as

$$\sum_{a \in I_+} \tilde{P}^{(\pm)}(a)^2 = \sum_{a \in I_-} \tilde{P}^{(\pm)}(a)^2 \qquad \text{(d)}$$

where $I_\pm$ = set of indices for the phase ±1 components.

The equilibrium distribution is given by the eigenvector of $\nu = 1$, i.e.,

$$P(a) = P^{(+)}(a) \qquad \text{or} \qquad \boldsymbol{P} = \boldsymbol{P}^{(+)}$$

Eq(A4.12) then gives

$$\tilde{P}^{(+)}(a) = \frac{P^{(+)}(a)}{\sqrt{P(a)}} = \sqrt{P(a)} \qquad \text{or} \qquad \tilde{\boldsymbol{P}}^{(+)} = \sqrt{\boldsymbol{P}} \qquad \text{(e)}$$

Eq(d) thus becomes

$$\sum_{a \in I_+} P(a) = \sum_{a \in I_-} P(a)$$

or (with $\boldsymbol{U}$ always trimmed to the proper dimension)

$$\boldsymbol{U}^T \boldsymbol{P}_+ = \boldsymbol{U}^T \boldsymbol{P}_-$$

Using eqs(A4.12m & 14m), we have

$$\boldsymbol{\Pi} \boldsymbol{P}^{(\pm)} = \pm \boldsymbol{P}^{(\pm)}$$

where

$$\boldsymbol{\Pi} = \begin{pmatrix} 0 & \boldsymbol{\pi} \\ \overline{\boldsymbol{\pi}} & 0 \end{pmatrix}$$

with

$$\boldsymbol{\pi} = \boldsymbol{D}^{1/2} \tilde{\boldsymbol{\pi}} \boldsymbol{D}^{-1/2} \qquad \overline{\boldsymbol{\pi}} = \boldsymbol{D}^{1/2} \tilde{\boldsymbol{\pi}}^T \boldsymbol{D}^{-1/2}$$

The eigenvectors are

$$\boldsymbol{P}^{(\pm)} = \begin{pmatrix} \boldsymbol{P}_{+}^{(\pm)} \\ \boldsymbol{P}_{-}^{(\pm)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{D}^{1/2} \boldsymbol{u} \\ \pm \boldsymbol{D}^{1/2} \boldsymbol{v} \end{pmatrix}$$

where

$$\boldsymbol{\pi} \boldsymbol{D}^{1/2} \boldsymbol{v} = \boldsymbol{D}^{1/2} \boldsymbol{u} \qquad \overline{\boldsymbol{\pi}} \boldsymbol{D}^{1/2} \boldsymbol{u} = \boldsymbol{D}^{1/2} \boldsymbol{v} \qquad \text{(e)}$$

$$\therefore \qquad \boldsymbol{\pi} \boldsymbol{D}^{1/2} \boldsymbol{v} = \boldsymbol{\pi} \overline{\boldsymbol{\pi}} \boldsymbol{D}^{1/2} \boldsymbol{u} = \boldsymbol{D}^{1/2} \boldsymbol{u} \qquad \rightarrow \qquad \boldsymbol{\pi} \overline{\boldsymbol{\pi}} = \boldsymbol{I}$$

$$\bar{\boldsymbol{\pi}}\, \boldsymbol{D}^{1/2}\, \boldsymbol{u} = \bar{\boldsymbol{\pi}}\, \boldsymbol{\pi}\, \boldsymbol{D}^{1/2}\, \boldsymbol{v} = \boldsymbol{D}^{1/2}\, \boldsymbol{v} \qquad \rightarrow \qquad \bar{\boldsymbol{\pi}}\, \boldsymbol{\pi} = \boldsymbol{I}$$

i.e.,

$$\bar{\boldsymbol{\pi}} = \boldsymbol{\pi}^{-1}$$

Eq(e) can also be written as

$$\boldsymbol{\pi}\, \boldsymbol{P}_{-}^{(-)} = -\boldsymbol{P}_{+}^{(-)} \qquad\qquad \bar{\boldsymbol{\pi}}\, \boldsymbol{P}_{+}^{(-)} = -\boldsymbol{P}_{-}^{(-)}$$

The left eigenvectors $\tilde{\boldsymbol{Q}}^{(\pm)}$ of $\tilde{\boldsymbol{\Pi}}$ are equal to the right eigenvectors $\tilde{\boldsymbol{P}}^{(\pm)}$.
Therefore, the left eigenvectors $\boldsymbol{Q}^{(\pm)}$ of $\boldsymbol{\Pi}$ are given by

$$\boldsymbol{Q}^{(\pm)\,T} = \tilde{\boldsymbol{P}}^{(\pm)\,T}\, \boldsymbol{D}^{1/2} = \left(\boldsymbol{P}_{+}^{(\pm)\,T},\ \ \boldsymbol{P}_{-}^{(\pm)\,T} \right) = \left(\boldsymbol{u}^{T}\, \boldsymbol{D}^{1/2},\ \ \pm \boldsymbol{v}^{T}\, \boldsymbol{D}^{1/2} \right)$$

Hence,

$$\begin{aligned} \boldsymbol{Q}^{(-)\,T}\, \boldsymbol{P} &= \left(\boldsymbol{u}^{T}\, \boldsymbol{D}^{1/2},\ \ -\boldsymbol{v}^{T}\, \boldsymbol{D}^{1/2} \right) \begin{pmatrix} \boldsymbol{D}^{1/2}\, \boldsymbol{u} \\ \boldsymbol{D}^{1/2}\, \boldsymbol{v} \end{pmatrix} \\ &= \boldsymbol{u}^{T}\, \boldsymbol{D}\, \boldsymbol{u} - \boldsymbol{v}^{T}\, \boldsymbol{D}\, \boldsymbol{v} \end{aligned}$$

Thus, contrary to Zinn-Justin’s statement, $\boldsymbol{Q}^{(-)}$ & $\boldsymbol{P}$ are not necessarily orthogonal.