Ex zero-range processes

$$\phi \xrightarrow{\kappa_0} S_1 \xrightarrow{\kappa_1} S_2 \rightarrow S_3 \cdots \cdots \rightarrow S_L \xrightarrow{\kappa_L} \phi$$

complex-balancing of terms in the master equation lead to

$$\kappa_0 P(N_{S_1}-1, N_{S_2}, \ldots N_{S_L}) = \kappa_1 N_{S_1} P(N_{S_1}, N_{S_2}, \ldots N_{S_L})$$

$$\kappa_1 P(N_{S_1}+1, N_{S_2}-1, N_{S_3} \cdots N_{S_L}) = \kappa_2 N_{S_2} P(N_{S_1}, N_{S_2} \cdots N_{S_L})$$

etc

which is consistent with the probability distribution

$$P(N_{S_1}, N_{S_2}, N_{S_3} \cdots N_{S_L}) = \frac{(x_{S_1})^{N_{S_1}} e^{-x_{S_1}}}{(N_{S_1})!} \frac{(x_{S_2})^{N_{S_2}} e^{-x_{S_2}}}{(N_{S_2})!} \cdots$$

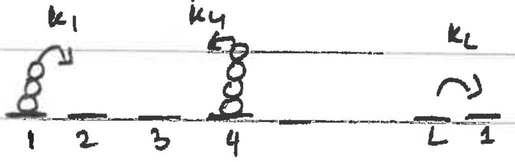
with the x's satisfying

$$\left.\begin{aligned} \kappa_0 &= \kappa_1 x_{S_1} \\ \kappa_1 x_{S_1} &= \kappa_2 x_{S_2} \\ &\vdots \\ \kappa_{L-1} x_{S_{L-1}} &= \kappa_L x_{S_L} \end{aligned}\right\} \text{etc}$$

So
$$x_{S_1} = \kappa_0/\kappa_1$$
$$x_{S_2} = \kappa_0/\kappa_2$$
$$\vdots$$
$$x_{S_L} = \kappa_0/\kappa_L$$

Ex. lets try the zero-range process with periodic boundary conditions!

ZRP with periodic boundary conditions



$$s_1 \to s_2 \to s_3 \cdots \to s_L \to s_1$$

· we could consider many variations such as

$$s_1 \rightleftarrows s_2 \rightleftarrows s_3 \cdots \rightleftarrows s_L$$

or

$$\begin{array}{c} \ \phi \\ \ \upharpoonleft\downharpoonright \\ s_1 \rightleftarrows s_2 \to s_3 \to s_4 \cdots \rightleftarrows s_L \\ \upharpoonleft\downharpoonright \\ \phi \end{array}$$

with sources & sinks, reversible or directional links etc.

Complex balance gives

$$n_{s_1} k_1 P(n_{s_1}, n_{s_2} \dots) = (n_{s_L}+1)\, k_L\, P(n_{s_1}-1, n_{s_2} \dots n_{s_L}+1)$$

$$n_{s_2} k_2 P(n_{s_1}, \dots) = (n_{s_1}+1)\, k_1\, P(n_{s_1}+1, n_{s_2}-1, \dots n_{s_L})$$

etc

which give us the condition

$$\left.\begin{array}{r} k_1 x_{s_1} = k_L x_{s_L} \\ k_2 x_{s_2} = k_1 x_{s_1} \\ \vdots \end{array}\right\}$$

if we input the ansatz $P(n_{s_1}, n_{s_2} \dots) = \frac{x_{s_1}^{n_{s_1}}}{(n_{s_1})!} \frac{x_{s_2}^{n_{s_2}}}{(n_{s_2})!} \dots \mathcal{N}$

$\mathcal{N}$ - normalization

In this case $\mathcal{N} = \frac{N!}{N^N}$ where $x_{s_1} + x_{s_2} + \dots x_{s_L} = N$

[because $\sum_{n_{s_1},\dots} \left[\frac{x_{s_1}^{n_{s_1}}}{n_{s_1}!} \dots\right]^{N^N} = \frac{N^N}{N!}$]

ACK result for more general kinetics

Instead of mass action, consider

$$2A \xrightarrow{k} A \quad \text{at rate} \quad k\,\theta_A(N_A)\,\theta_A(N_A-1)$$

or

$$2A + B \xrightarrow{\bar{k}} C \quad \text{at rate} \quad \bar{k}\,\theta_A(N_A)\,\theta_A(N_A-1)\,\theta_B(N_B)$$

with $\theta_i(x) = 0$ for $x \le 0$

ACK prove that if the mass-action CRN, deterministically modeled by the same rate constants has a complex-balanced equilibrium, then the stochastic system admits the stationary distribution

$$P(n_A, n_B \cdots) = M \prod_{i=1}^{m} \frac{x_i^{n_i}}{\prod_{j=1}^{n_i} \theta_i(j)}$$

where $M > 0$ is a normalizing constant, provided the above is summable.

Conditions for Factorized steady states

- Partial Balance (Kelly[1])
- Product form Queuing networks [2]
- Chipping condition of Evans, Majumdar and Zia [3]: holds also for continuous masses and discreet time dynamics
- Pair factorised steady states ? [4]

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[1] Frank. P. Kelly, *Reversibility and Stochastic Networks*, Wiley Series in Prob. and Math Stat. (1979)

[2] R. Nelson, ACM Computing Surveys **25**, 339 (1993)

[3] J. Phys. A: Math Gen **37**, L275 (2004), J. Stat. Mech: Theory Exp, L10001 (2004)

[4] Evans, Hanney and Majumdar, Phys. Rev. Lett. **97**, 010602 (2006)

$\delta \neq 0$ networks

$$A \underset{\epsilon}{\overset{\alpha}{\rightleftharpoons}} 2A \underset{\beta}{\overset{\epsilon}{\rightleftharpoons}} 3A$$

[don't confuse species A with our A matrix!]

$$\delta = \dim \left[\mathrm{Im}\, A \cap \ker Y \right]$$

if $\delta = 0 \Rightarrow (\mathrm{Im}\, A \cap \ker Y)^{\perp} = \mathbb{R}^c$

if $\delta \neq 0 \Rightarrow (\mathrm{Im}\, A \cap \ker Y)^{\perp} \neq \mathbb{R}^c$

& we are not guaranteed that any vector in $\mathbb{R}^c$, such as $\bar{\Psi}$, can be described by our scheme.

$$\frac{\partial P(n_A)}{\partial t} = \alpha P(n_A-1)(n_A-1) - \alpha P(n_A) n_A$$
$$+ \epsilon P(n_A+1)(n_A+1) n_A - \epsilon n_A (n_A-1) P(n_A)$$
$$+ \epsilon P(n_A-1)(n_A-1)(n_A-2) - \epsilon P(n_A) n_A (n_A-1)$$
$$+ \beta P(n_A+1)(n_A+1) n_A (n_A-1)$$
$$- \beta P(n_A) n_A (n_A-1)(n_A-2)$$

Let's try to write an eqn of the sort

$$\frac{\partial \phi}{\partial t} = -\mathcal{L} \bar{\Phi}$$

we can do this for $\phi = \sum_{n_a} P(n_a) z^{n_a}$

$$\frac{\partial \phi}{\partial t} = \alpha \sum_{n_A} z^{n_A} \left[P(n_A-1)(n_A-1) - n_A P(n_A) \right]$$
$$+ \epsilon \sum_{n_A} z^{n_A} \left[P(n_A+1) n_A (n_A+1) - n_A (n_A-1) P(n_A) \right]$$
$$+ \epsilon \sum_{n_A} z^{n_A} \left[P(n_A-1)(n_A-1)(n_A-2) - P(n_A) n_A (n_A-1) \right]$$
$$+ \beta \sum_{n_A} z^{n_A} \left[P(n_A+1)(n_A+1) n_A (n_A-1) - P(n_A) n_A (n_A-1)(n_A-2) \right]$$

- we can do the sum over n_A's ~~also~~ in a similar manner to how we wrote eqns for the averages (directly from the master eqn.)

Consider

$$\sum_{n_A} \alpha z^{n_A} P(n_A-1)(n_A-1) - \sum \alpha z^{n_A} P(n_A) n_A$$

$$\downarrow$$

$$\sum_{n_A} \alpha \left[z^{n_A+1} P(n_A) n_A - z^{n_A} P(n_A) n_A \right]$$

$$\downarrow$$

$$\sum_{n_A} \alpha (z-1) z^{n_A} P(n_A) n_A$$

$$= \alpha (z-1) z \frac{\partial}{\partial z} \phi$$

Similarly

$$\sum z^{n_A} \epsilon \left[P(n_A+1)(n_A+1) n_A - P(n_A) n_A (n_A-1) \right]$$

$$\downarrow$$

$$\sum z^{n_A-1} \epsilon \left[P(n_A) n_A (n_A-1) - P(n_A) n_A (n_A-1) \right]$$

$$\downarrow$$

$$\epsilon \left(\frac{1}{z} - 1 \right) z^2 \frac{\partial^2}{\partial z^2} \phi$$

If we go through this procedure, we get

$$\frac{\partial \phi}{\partial t} = -\left\{ (1-z) \left[\alpha z \frac{\partial}{\partial z} - \epsilon (1-z) z \frac{\partial^2}{\partial z^2} - \beta z^2 \frac{\partial^3}{\partial z^3} \right] \right\} \phi$$

$\mathcal{L}$ has a well-known representation, due to Doi, in terms of raising & lowering operators.
The Doi algebra uses the following correspondence

(1) $z \to a^+$ $\qquad \frac{\partial}{\partial z} \to a$

(2) $[a, a^+] = 1$

(3) $1 \to |0\rangle$

(4) $a^{+n_A} |0\rangle \equiv |n_A\rangle$

[can be done for an arbitrary # of species]

$\phi(z)$ becomes $\sum_{n_A} z^{n_A} P(n_A) \to \sum P(n_A) |n_A\rangle$
$\equiv |\varphi\rangle$

$$\frac{\partial |\varphi\rangle}{\partial t} = -\mathcal{L}(a, a^+) |\varphi\rangle$$

By this correspondence

$$\mathcal{L} = (1 - a^+)(a^+ a)\left[(\alpha - \epsilon a) + (a^+ a - 1)(\epsilon - \beta a)\right]$$

we can define $\psi^+ \equiv [a^+, a^{+2}, a^{+3}]$
$$\psi \equiv \begin{bmatrix} a \\ a^2 \\ a^3 \end{bmatrix}$$

$\Rightarrow$ $-\mathcal{L} = \psi^+ A \psi$ $\to$ generally true for mass-action kinetics

Moment hierarchies

$$A \to \begin{array}{c} A \\ 2A \\ 3A \end{array}\begin{bmatrix} -\alpha & \epsilon & 0 \\ \alpha & -2\epsilon & \beta \\ 0 & \epsilon & -\beta \end{bmatrix}$$

$$Y = [1 \;\; 2 \;\; 3] \; ; \; Y^{\underline{2}} \to [0, 2, 6] \; ; \; Y^{\underline{3}} \to [0, 0, 6]$$

$$Y^{\underline{4}} \to [0, 0, 0]$$

$$\bar{\Psi} \to \begin{bmatrix} a \\ a^2 \\ a^3 \end{bmatrix} \quad \text{which translates to} \quad \begin{bmatrix} \langle n_A \rangle \\ \langle n_A(n_A-1) \rangle \\ \langle n_A(n_A-1)(n_A-2) \rangle \end{bmatrix}$$

std st eqn. here implies

$$0 = k\,[\alpha, 0, -\beta] \begin{bmatrix} \langle n_A^{\underline{k}} \rangle \\ \langle n_A^{\underline{k+1}} \rangle \\ \langle n_A^{\underline{k+2}} \rangle \end{bmatrix} + \frac{k(k-1)}{2}\,[2\alpha, 2\epsilon, -4\beta] \begin{bmatrix} \langle n_A^{\underline{k-1}} \rangle \\ \langle n_A^{\underline{k}} \rangle \\ \langle n_A^{\underline{k+1}} \rangle \end{bmatrix} + \frac{k(k-1)(k-2)}{6}\,[0, 6\epsilon, -6\beta] \begin{bmatrix} \langle n_A^{\underline{k-2}} \rangle \\ \langle n_A^{\underline{k-1}} \rangle \\ \langle n_A^{\underline{k}} \rangle \end{bmatrix}$$

$$n_A^{\underline{k}} = n_A(n_A-1)\cdots(n_A-k+1)$$

$\downarrow$ factorial moments $\equiv \dfrac{n_A!}{(n_A-k)!}$

for all $1 \le k \le \infty$

If we define $R_k \equiv \dfrac{\langle n_A^{\underline{k}} \rangle}{\langle n_A^{\underline{k-1}} \rangle}$, we get a recursion relation

$$R_k = \frac{(k-1)\left[\alpha/\beta + \epsilon/\beta\,(k-2)\right]}{\left[(k-1)\left[2R_{k+1} + (k-2) - \frac{\epsilon}{\beta}\right] + R_{k+2}R_{k+1} - \frac{\alpha}{\beta}\right]}$$