Math 613 * Fall 2019 * Probability Generating Function * Victor Matveev

1. **(18pts)** Consider the continuous-time stochastic process describing the following chemical reaction:

$$\left\{A \xrightarrow{k_D} \varnothing;\quad \varnothing \xrightarrow{k_B} A\right\}$$

a) Write down the Chemical Master Equations (CME).

$$\begin{cases} \dfrac{dp_0}{dt} = -k_B p_0 + k_D p_1 \\ \dfrac{dp_n}{dt} = k_B\left[p_{n-1} - p_n\right] + k_D\left[(n+1)p_{n+1} - np_n\right] \quad (n>0) \end{cases}$$

b) Find the equation for the evolution of the second moment, $\dfrac{d\langle n^2\rangle}{dt}$.

$$\frac{d}{dt}\sum_{n=0}^{\infty} n^2 p_n = k_B\left[\sum_{n=1}^{\infty} n^2 p_{n-1} - \sum_{n=0}^{\infty} n^2 p_n\right] + k_D\left[\sum_{n=0}^{\infty} n^2 (n+1) p_{n+1} - \sum_{n=0}^{\infty} n^3 p_n\right]$$

$$\Rightarrow \frac{d}{dt}\sum_{n=0}^{\infty} n^2 p_n = k_B\left[\sum_{m=0}^{\infty} (m+1)^2 p_m - \sum_{n=0}^{\infty} n^2 p_n\right] + k_D\left[\sum_{m=0}^{\infty} (m-1)^2 m p_m - \sum_{n=0}^{\infty} n^3 p_n\right]$$

$$\Rightarrow \frac{d}{dt}\langle n^2\rangle = k_B\left[\left\langle (n+1)^2\right\rangle - \left\langle n^2\right\rangle\right] + k_D\left[\left\langle n(n-1)^2\right\rangle - \left\langle n^3\right\rangle\right]$$

$$= k_B\left[2\langle n\rangle + 1\right] + k_D\left[\left\langle n^3 - 2n^2 + n\right\rangle - \left\langle n^3\right\rangle\right] = \boxed{k_B\left[2\langle n\rangle + 1\right] + k_D\left[-2\left\langle n^2\right\rangle + \langle n\rangle\right]}$$

c) Find the partial differential equation (PDE) for the probability-generating function, $F(z,t) = \sum_{n=0}^{\infty} p_n(t) z^n$

$$\frac{d}{dt}\sum_{n=0}^{\infty} z^n p_n = k_B\left[\sum_{n=1}^{\infty} z^n p_{n-1} - \sum_{n=0}^{\infty} z^n p_n\right] + k_D\left[\sum_{n=0}^{\infty} (n+1) z^n p_{n+1} - \sum_{n=0}^{\infty} n z^n p_n\right]$$

$$\Rightarrow \frac{\partial F}{\partial t} = k_B\left[\sum_{m=0}^{\infty} z^{m+1} p_m - F(z)\right] + \frac{k_D}{2}\left[\sum_{m=1}^{\infty} m z^{m-1} p_m - z\frac{\partial F}{\partial z}\right]$$

$$\Rightarrow \frac{\partial F}{\partial t} = k_B\left[zF - F\right] + k_D\left[\frac{\partial F}{\partial z} - z\frac{\partial F}{\partial z}\right] \quad \Rightarrow \quad \boxed{\frac{\partial F}{\partial t} = (z-1)\left[k_B F - k_D\frac{\partial F}{\partial z}\right]}$$

d) Find the equilibrium probability distribution. Make sure that completeness is satisfied: $\sum_{n=0}^{\infty} p_n = 1$

$$\frac{\partial F_{eq}}{\partial t} = 0 \;\Rightarrow\; k_B F_{eq} - k_D \frac{dF_{eq}}{dz} = 0 \;\Rightarrow\; \frac{dF_{eq}(z)}{dz} = \frac{k_B}{k_D}F(z) \;\Rightarrow\; \boxed{F_{eq}(z) = Ce^{\alpha z}} \quad \text{where } \alpha = \frac{k_B}{k_D}$$

$$\sum_{n=0}^{\infty} p_n = 1 \Rightarrow F_{eq}(1) = Ce^{\alpha} = 1 \Rightarrow C = e^{-\alpha} \Rightarrow F_{eq}(z) = e^{-\alpha}\, e^{\alpha z} = e^{-\alpha} \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} z^n \Rightarrow \boxed{p_n^{eq} = \frac{\alpha^n}{n!} e^{-\alpha}}$$

Of course, we obtained the same result directly from the CME system

Finally, let's solve for the probability generating function:

$$\tau = k_D t \Rightarrow \boxed{\frac{\partial F}{\partial \tau} = (z-1)\left[\alpha F - \frac{\partial F}{\partial z}\right]} \quad \text{where} \quad \alpha = \frac{k_B}{k_D}$$

$$F(z,\tau) = e^{\alpha z} G(z,\tau) \Rightarrow \frac{\partial G}{\partial \tau} e^{\alpha z} = (z-1)\left[\alpha G e^{\alpha z} - \alpha G e^{\alpha z} - \frac{\partial G}{\partial z} e^{\alpha z}\right] \Rightarrow \boxed{\frac{\partial G}{\partial \tau} + (z-1)\frac{\partial G}{\partial z} = 0}$$

Solve by the method of characteristic:

$$\frac{dz}{d\tau} = z-1 \Rightarrow \frac{dz}{z-1} = d\tau \Rightarrow \ln\frac{z-1}{z_0-1} = \tau \Rightarrow z-1 = (z_0-1)\exp(\tau) \Rightarrow z_0 - 1 = (z-1)\exp(-\tau)$$

$$\Rightarrow \begin{cases} G(z,t) = G_0(z_0(z,t)) = F_0(z_0)\, e^{-\alpha z_0} \\ \qquad \text{where} \\ z_0 = 1 + (z-1)\exp(-\tau) \end{cases}$$

$$F(z,\tau) = G(z,\tau)\exp(\alpha z)$$

$$= F_0(z_0)\,\exp(-\alpha z_o + \alpha z) = F_0\left(1 + (z-1)e^{-\tau}\right)\exp\left(-\alpha\left(1 + (z-1)e^{-\tau}\right) + \alpha z\right)$$

$$= \boxed{F_0\left(1 + (z-1)e^{-\tau}\right)\exp\left(-\alpha(z-1)\left(e^{-\tau} - 1\right)\right)} = F_0\left(1 + (z-1)e^{-k_D t}\right)\exp\left(-\alpha(z-1)\left(e^{-k_D t} - 1\right)\right)$$

Example: m particles with probability =1 at time $t = 0$:

$$F_0(z_0) = z_0^m \Rightarrow F(z,t) = \left(1 + (z-1)e^{-k_D t}\right)^m \exp\left(-\alpha(z-1)\left(e^{-k_D t} - 1\right)\right)$$