2 Problem 2

Consider the process:

$$\mathrm{X} + \mathrm{R} \xrightarrow{k} \mathrm{X} + \mathrm{X}$$

where X and R are molecules of two different substances that react with each other to give rise to two molecules of the X type. If $\hat{n}$ is a random variable that gives the total number of X particles and $\hat{m}$ a second random variable that gives the total number of R particles, the dynamics is such that the total number of particles is conserved: $\hat{n} + \hat{m} = N \ \forall t$. Write the Master equation for the probability of having n particles of type X at time t, $p_{\hat{n}}(n,t)$. Analyze the mean number of particles as a function of time using a (i) mean-field and (ii) a Gaussian approximation. What are the mean differences and similarities you observe between this scenario and the one studied in Problem 1. Discuss your results.

$$\frac{dP(n,t)}{dt} = \sum_{\ell} \left(E^{\ell} - 1\right)\left[\Omega_{n \to n-\ell} P(n,t)\right]$$

$$\Omega_{n\to n-\ell} \neq 0 \iff \ell = -1 \Rightarrow \Omega_{n \to n+1} = \begin{cases} knm = Kn(N-n), & n \leq N \\ 0, & n > N \end{cases}$$

$$\Rightarrow \frac{dP(n,t)}{dt} = \left(E^{-1} - 1\right)\left[Kn(N-n)P(n,t)\right].$$

$$\therefore \boxed{\frac{d}{dt} P(n,t) = K(n-1)(N-n+1)P(n-1,t) - Kn(N-n)P(n,t)}$$

* Mean Field approximation:

$$\frac{d}{dt}\langle n(t)\rangle = -\langle -1 \cdot \Omega_{n\to n+1}\rangle = \langle Kn(t)(N-n(t))\rangle =$$

$$= KN\langle n(t)\rangle - K\langle n^2(t)\rangle \overset{\text{M.F.A.}}{=} KN\langle n(t)\rangle - K\langle n(t)\rangle^2. \ (= F(\langle n(t)\rangle))$$

From Problem 1, we already know this equation has a solution:

$$\boxed{\langle n(t)\rangle = \frac{KN n(0) e^{KNt}}{KN - Kn(0)\left(1 - e^{KNt}\right)} = \frac{N n(0) e^{KNt}}{N - n(0)\left(1-e^{KNt}\right)}}.$$

And we know the state for $t \to \infty$: As both k and N are positive, we have $kN > 0$ so

$$\lim_{t\to\infty} \langle n(t) \rangle = \lim_{t\to\infty} \frac{N n(0)}{(N-n(0))e^{-kNt} + n(0)} = \frac{N n(0)}{n(0)} = \underline{N}.$$

That means $n=N, m=0$ will always be the final state of the system, at least in the M.F. approximation.

Notice that this does not mean $\langle n(t) \rangle = N$ is the only equilibrium point of the system. We can also have $\langle n(t) \rangle = 0$:

$F(0) = kN \cdot 0 - k \cdot 0 = 0,$

but we can show it's unstable: $F'(x)\big|_{x=0} = (kN - 2kx)\big|_{x=0} = kN > 0.$

And $\langle n(t) \rangle = N$ is of course a stable fixed point:

$F(N) = kN \cdot N - k \cdot N^2 = 0;\ F'(x)\big|_{x=N} = (kN - 2kx)\big|_{x=N} = -kN < 0.$

* Gaussian Approximation

- $$\boxed{\frac{d}{dt}\langle n(t) \rangle = kN\langle n(t) \rangle - k\langle n^2(t) \rangle}$$

- $$\frac{d}{dt}\langle n^2(t) \rangle = \sum_{\ell} \langle \ell(\ell - 2n)\Omega_{n\to n-\ell} \rangle = \langle -1(-1-2n)kn(N-n) \rangle =$$

$$= \langle (1+2n)kn(N-n) \rangle = k\langle n(N-n) \rangle + 2k\langle n^2(N-n) \rangle =$$

$$= kN\langle n \rangle - k\langle n^2 \rangle + 2kN\langle n^2 \rangle - 2k\langle n^3 \rangle$$

$* \; G.A.: \langle n^3\rangle = 3\langle n\rangle\langle n^2\rangle - 2\langle n\rangle^3$

$$\therefore \boxed{\frac{d}{dt}\langle n^2(t)\rangle = KN\langle n(t)\rangle + K(2N-1)\langle n^2(t)\rangle + 4K\langle n(t)\rangle^3 - 6K\langle n(t)\rangle\langle n^2(t)\rangle}$$

Take $\langle n(t)\rangle \to x$, $\langle n^2(t)\rangle \to y$:

$$\frac{dx}{dt} = KNx - Ky = F(x,y)$$

$$\frac{dy}{dt} = KNx + K(2N-1)y + 4Kx^3 - 6Kxy = g(x,y)$$

$$\frac{dx}{dt} = 0 \Rightarrow y = Nx$$

$$\frac{dy}{dt} = Nx + (2N-1)Nx + 4x^3 - 6Nx^2 = 0$$

1^{st} solution: $\boxed{y = x = 0}$, other solutions:

$$4x^2 - 6Nx + \cancel{N} + 2N^2 - \cancel{N} = 0 \Rightarrow 2x^2 - 3Nx + N^2 = 0 \Rightarrow$$

$$\Rightarrow x_\pm = \frac{3N \pm \sqrt{9N^2 - 8N^2}}{4} = \frac{3 \pm 1}{4} N \Rightarrow \boxed{\begin{array}{l} x_+ = N \Rightarrow y_+ = N^2 \\ x_- = N/2 \Rightarrow y_- = N^2/2 \end{array}}$$

$*$ Stability: $\cdot \; \frac{\partial F}{\partial x} = KN$; $\cdot \; \frac{\partial F}{\partial y} = -K$;

$\cdot \; \frac{\partial g}{\partial x} = KN + 12Kx^2 - 6Ky$; $\cdot \; \frac{\partial g}{\partial y} = K(2N-1) - 6Kx$

$$\Rightarrow M = \begin{pmatrix} KN & -K \\ KN + 12Kx^2 - 6Ky & K(2N-1) - 6Kx \end{pmatrix}$$

$$* \; y = x = 0 \Rightarrow M = \begin{pmatrix} kN & -k \\ kN & k(2N-1) \end{pmatrix} \Rightarrow \operatorname{Tr} M = 3kN - k = $$

$$= \underline{k(3N-1) > 0}.$$

$$\cdot \det M = k^2 N(2N - \cancel{1}) + \cancel{k^2 N} = \underline{2k^2 N^2 > 0}.$$

$$\therefore \boxed{y = x = 0 \text{ is unstable.}}$$

$$* \; x = N, \; y = N^2 \Rightarrow M = \begin{pmatrix} kN & -k \\ kN + 12kN^2 - 6kN^2 & k(2N-1) - 6kN^2 \end{pmatrix} \Rightarrow$$

$$\Rightarrow \operatorname{Tr} M = 2kN - k - 6kN^2$$

$$\cdot \; -6kN^2 + 2kN - k = 0 \Rightarrow N = \frac{-2k \pm \sqrt{4k^2 - 24k^2}}{-12k} \Rightarrow \underline{\operatorname{Tr} M < 0}$$

$$\det M = 2k^2N^2 - \cancel{k^2N} - 6k^2N^3 + \cancel{k^2N} + 12kN^2 - 6kN^2 =$$

$$= -6k^2N^3 + 2k(1+3k)N^2 = N^2\left[2k(1+3k) - 6k^2N\right] =$$

$$= N^2\left[2k + 6k^2 - 6k^2N\right] < 0 \Rightarrow 6k^2N > 6k^2 + 2k \Rightarrow N > \frac{6k+2}{6k}$$

$$\therefore \boxed{x = N, \; y = N^2 \text{ is stable if } N > \frac{6k+2}{6k}.}$$

$$* \; x = N/2, \; y = N^2/2 \Rightarrow M = \begin{pmatrix} kN & -k \\ kN + \cancel{3kN^2} - \cancel{3kN^2} & k(2N-1) - 3kN \end{pmatrix} \Rightarrow$$

$$\Rightarrow \operatorname{Tr} M = 3kN - k - 3kN = \underline{-k < 0}$$

- $\det M = 2K^2N^2 - \cancel{K^2N} - 3K^2N^2 + \cancel{K^2N} = -K^2N^2 < 0$

$\therefore$ M has one positive and one negative eigenvalue. Therefore, $x = N/2$, $y = N^2/2$ is a saddle point.

Comparing to Problem 1, we have very similar approximation equations, even having a different Master Equation. For Problem 2, we have less parameters, so the problem is much more tractable, analytically.

It's interesting to notice that, in Problem 2, the trivial fixed point is always unstable in both approximations, and we also have a non trivial fixed point that is always a saddle point.

Lastly, as in Problem 1, for the gaussian approximation, we can have cases in which neither fixed point is stable, so the solution may diverge.