TUTORIAL 10

7CCMCS04
A. ANNIBALE AND G. SICURO

Problem 10.1 Consider the reaction of annihilation

$$\mathrm{A} + \mathrm{A} \to \varnothing$$

and let us study the probability law of the number N_t of particles at time t.

a. Explain why the master equation for the probability $P_n(t) = \mathbb{P}[\mathsf{N}_t = n]$ can be written as

$$\dot{P}_n(t) = \frac{1}{2V}(\mathcal{E}^2 - 1)n(n-1)P_n(t)$$

where the action of the raising operator $\mathcal{E}$ on a function of n is

$$\mathcal{E}f(n) = f(n+1)$$

and the prefactor V^{-1}, is needed to recover the proper rate equation for the density $\rho(t)$ of particles.

b. Assume that fluctuations of n about the deterministic value ρV are small so that we can write

$$n = V\rho + \sqrt{V}\eta$$

where η is a stochastic variable. We also write $P_n(t) = \Pi(\xi, t)$. By considering the effect that $\mathcal{E}$ has on n deduce its effect on η and η^2, hence deduce that

$$\mathcal{E} = 1 + \frac{1}{\sqrt{V}}\frac{\partial}{\partial \eta} + \frac{1}{2V}\frac{\partial^2}{\partial \eta^2} + \dots$$

c. By observing that derivatives are taken with n held constant, show that

$$\dot{P}_n = \frac{\partial \Pi}{\partial t} - \sqrt{V}\dot{\rho}\frac{\partial \Pi}{\partial \eta}$$

d. Perform an expansion of the master equation in inverse powers of the volume and show that orders $\sqrt{V}$ give

$$\dot{\rho} = -\rho^2$$

and orders V^0 gives the Fokker-Planck equation

$$\frac{\partial \Pi}{\partial t} = 2\rho\frac{\partial(\eta\Pi)}{\partial \eta} + \rho^2\frac{\partial^2 \Pi}{\partial \eta^2}$$

Date: February 13, 2025.

e. Use the Fokker-Planck equation to find the equation for the first two moments $M_k = \int \mathrm{d}\,\eta \eta^k \Pi(\xi, t)$, with $k = 1, 2$. Solve them and use the results to show that the relative fluctuation is

$$\frac{\sqrt{\mathrm{Var}[\mathsf{N}_t]}}{\mathbb{E}[\mathsf{N}_t]} = \sqrt{\frac{2}{3}\frac{1 + t - (1+t)^{-2}}{V}}.$$

Reflect on the behavior of the relative fluctuations with time and with n.

✎ **Problem 10.2** Consider a system of N particles of a single species X which evolve stochastically. Each X particle decays with unit rate

$$\mathrm{X} \to 0 \quad \text{with rate } 1$$

a. Write the Master equation for the probability density $P_n(t)$ to have $\mathsf{N}_t = n$ particles X at time t and calculate the average number of particles $\mathbb{E}[\mathsf{N}_t] = \sum_{n=1}^{\infty} n\, P_n(t)$ at time t.

b. Assume that a decay occurs at time t and let us call T the time to wait until the next event. Calculate the probability $\mathbb{P}[\tau \le \mathsf{T} \le \tau + \mathrm{d}\,t | \mathsf{N}_t = n]$ that, given $\mathsf{N}_t = n$, the next decay occurs in the time interval $[t+\tau, t+\tau+\mathrm{d}\,t)$, in the limit $\mathrm{d}\,t \to 0$. Hence show that the probability density of the waiting times T between successive events, given the number n of particles, is $\rho_n(t) = n\,\mathrm{e}^{-n\tau}$.
Hint: It is convenient to partition the time interval τ in many small intervals of duration $\Delta \to 0$ and use $1 - x \simeq \mathrm{e}^{-x}$ for $x \to 0$.

c. One can simulate this system via the following Gillespie algorithm:
1 Initialize time and number of particles: $t = 0$, $n = N$;
2 While $n > 0$ do:
 2.1 Generate a random number $r \in (0, 1)$;
 2.2 Set $\tau = \frac{1}{n} \ln \frac{1}{r}$;
 2.3 Update time and number of particles: $t = t + \tau$; $n = n - 1$;

Justify this algorithm.
Hint: You may find useful to note that $\int_0^\infty \mathrm{d}\,\tau\, n\,\mathrm{e}^{-n\tau} = 1$.

d. Assume that the system evolves in a large volume V. By carrying out a Kramers–Moyal expansion of the master equation in inverse powers of V, show that the Fokker-Planck equation for the evolution of the distribution $q(x, t)$ of the concentration $\mathsf{X}_t = {}^{\mathsf{N}_t}/_V$ of particles, is

$$\partial_t q(x,t) = \frac{\partial}{\partial x}[xq(x,t)] + \frac{1}{2V}\frac{\partial^2}{\partial x^2}[xq(x,t)]$$

e. Use the Fokker-Planck equation for $q(x, t)$ to derive the equation of motion for the average concentration $\mathbb{E}[\mathsf{X}_t] = \int \mathrm{d}\,x\, xq(x, t)$ and for the fluctuations about the average $\sigma^2(t) = \mathrm{Var}[\mathsf{X}_t]$ and solve them for the initial condition $\mathsf{X}_0 = {}^{N}/_{V}$.

✎ **Problem 10.3** Solve the heat equation

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2}$$

with absorbing boundary conditions in 0 and L.