TUTORIAL 10 — SOLUTIONS

7CCMCS04
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Problem 10.1

a. Applying the definition of $\mathcal{E}$:

$$\dot{P}_n = \frac{(n+2)(n+1)P_{n+2} - n(n-1)P_n}{2V}$$

the gain term is due to the fact that any of the $n+2$ particles interacts with any other particle and both annihilate. The loss term is due to the same process starting with n particles.

b. We have that $\mathcal{E}n = n+1$ and $\mathcal{E}n^2 = (n+1)^2$. Hence we can write

$$\mathcal{E}\eta = \eta + \frac{1}{\sqrt{V}} \qquad \mathcal{E}\eta^2 = \left(\eta + \frac{1}{\sqrt{V}}\right)^2 = \eta^2 + \frac{2}{\sqrt{V}}\eta + \frac{1}{V}$$

so

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

c. + d. From $\mathrm{d}\,n = V\,\mathrm{d}\,\rho + \sqrt{V}\,\mathrm{d}\,\eta$, at constant n $\mathrm{d}\,\eta = -\sqrt{V}\,\mathrm{d}\,\rho$ so

$$\frac{\mathrm{d}\,\Pi}{\mathrm{d}\,t} = \frac{\partial \Pi}{\partial t} + \frac{\partial \Pi}{\partial \eta}\frac{\mathrm{d}\,\eta}{\mathrm{d}\,t} = \frac{\partial \Pi}{\partial t} - \sqrt{V}\dot{\rho}\frac{\partial \Pi}{\partial \eta}.$$

Next we calculate $\mathcal{E}^2 = 1 + 2V^{-1/2}\frac{\partial}{\partial \eta} + 2V^{-1}\frac{\partial^2}{\partial \eta^2} + \dots$ so to orders V^{-1}

$$\mathcal{E}^2 - 1 = 2V^{-1/2}\frac{\partial}{\partial \eta} + 2V^{-1}\frac{\partial^2}{\partial \eta^2}.$$

Also observing that

$$n^2 - n = (V\rho)^2 + 2V^{3/2}\rho\eta + \dots$$

and substituting into the master equation we get

$$\frac{\partial \Pi}{\partial t} - \sqrt{V}\dot{\rho}\frac{\partial \Pi}{d\eta} = \frac{1}{2V}\left(\frac{2}{\sqrt{V}}\frac{\partial}{\partial \eta} + \frac{2}{V}\frac{\partial^2}{\partial \eta^2}\right)[(V\rho)^2 + 2V^{3/2}\rho\eta].$$

Collecting terms orders $\sqrt{V}$ we have the equation for the non-fluctuating part ρ:

$$\dot{\rho}\frac{\partial \Pi}{\partial \eta} = -\rho^2\frac{\partial \Pi}{\partial \eta} \Rightarrow \dot{\rho} = -\rho^2,$$

and to V^0 we have the Fokker-Planck equation (FPE) for the fluctuations η

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

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Solving the equation for ρ we have

$$\dot{\rho} = -\rho^2 \Rightarrow \rho = \frac{1}{1+t}$$

e. We can get M_1 by multiplying the FPE by η and integrating over η, obtaining $\dot{M}_1 = -2\rho M_1$, where we have solved the integral over η on the right-hand side by parts. Multiplying the FPE by η^2 and integrating over η we have instead

$$\dot{M}_2 = -4\rho M_2 + 2\rho^2$$

The equation for M_1 gives $M_1(t) = 0$ because $M_1(0) = 0$ (since the initial condition is deterministic). The equation for M_2 can be solved by integrating factors. For the initial condition $M_2(0) = 0$ (following again from the deterministic initial condition $\Pi(\eta, 0) = \delta(\eta)$) we have

$$M_2 = 2\frac{(1+t)^{-1} + (1+t)^{-4}}{3}$$

Finally one has $\mathbb{E}[\mathsf{N}_t] = \rho V$ and $\mathrm{Var}[\mathsf{N}_t] = \mathbb{E}[(\mathsf{N}_t - \rho V)^2] = V\mathbb{E}[\eta^2] = VM_2$ from which the result follows

$$\frac{\mathrm{Var}[\mathsf{N}_t]}{\mathbb{E}[\mathsf{N}_t]} = \frac{M_2}{V\rho^2}.$$

Problem 10.2

a. The master equation for $P_n(t)$ has a gain term from transitions from state $n+1$ to n (with rate $n+1$ as each of the $n+1$ decays with unit rate) and a loss term from transitions from state n to $n-1$ (with rate n as each of the n decays with unit rate)

$$\dot{P}_n = -nP_n + (n+1)P_{n+1}.$$

Multiplying times n and summing over n we have

$$\begin{aligned}\partial_t \mathbb{E}[\mathsf{N}_t] &= -\sum_{n=1}^{\infty} n^2 P_n(t) + \sum_{n=1}^{\infty} n(n+1)P_{n+1} = -\mathbb{E}[\mathsf{N}_t^2] + \sum_{n=1}^{\infty}(n-1)nP_n \\ &= -\mathbb{E}[\mathsf{N}_t^2] + \mathbb{E}[\mathsf{N}_t^2] - \mathbb{E}[\mathsf{N}_t] = -\mathbb{E}[\mathsf{N}_t].\end{aligned}$$

For the initial condition $P_n(0) = \delta_{n,N}$ i.e. $\mathbb{E}[\mathsf{N}_0] = N$, $\mathbb{E}[\mathsf{N}_t] = N\,\mathrm{e}^{-t}$.

b. $\mathbb{P}[\tau \le \mathsf{T} \le \tau + \mathrm{d}\,t | \mathsf{N}_t = n] = \mathbb{P}[\mathsf{N}_{t+\tau} = n|\mathsf{N}_t = n] \times \mathbb{P}[\mathsf{N}_{t+\tau+\mathrm{d}\,t} = n|\mathsf{N}_{t+\tau} = n] = \mathbb{P}[\mathsf{N}_{t+\tau} = n|\mathsf{N}_t = n] \times n\,\mathrm{d}\,t$. We partition the interval $(t, t+\tau]$ in T small intervals $\mathrm{d}\,t_i$ with $i = 1,\dots,T$ and $\tau = \sum_{i=1}^{T} \mathrm{d}\,t_i$. Then

$$\mathbb{P}[\mathsf{N}_{t+\tau} = n|\mathsf{N}_t = n] = \prod_{i=1}^{T}(1 - n\,\mathrm{d}\,t_i) \simeq \prod_{i=1}^{T} \mathrm{e}^{-n\,\mathrm{d}\,t_i} = \mathrm{e}^{-n\sum_{i=1}^{T}\mathrm{d}\,t_i} = \mathrm{e}^{-n\tau}$$

where we used $\mathrm{d}\,t_i \to 0$. Hence the probability density of waiting times between two successive events is

$$\mathbb{P}[\tau \le \mathsf{T} \le \tau + \mathrm{d}\,t|\mathsf{N}_t = n] = n\,\mathrm{e}^{-n\tau}\,\mathrm{d}\,\tau \to \rho_n(\tau) = n\,\mathrm{e}^{-n\tau}\,.$$

c. The probability density is normalised to one, i.e., $\int_0^\infty \rho_n(\tau)\,\mathrm{d}\,\tau' = 1$, hence $0 < \int_0^\tau \rho_n(\tau')\,\mathrm{d}\,\tau' < 1 \;\forall\; 0 < \tau < \infty$. We set

$$r = \int_0^\tau \rho_n(\tau')d\tau' = n\int_0^\tau \mathrm{e}^{-n\tau'}\,\mathrm{d}\,\tau' = 1 - \mathrm{e}^{-n\tau} \Rightarrow \tau = \frac{1}{n}\ln\frac{1}{1-r}.$$

Since $r \in (0,1)$, $1-r \in (0,1)$. Hence the algorithm generates, at each iteration, the time τ that needs to be waited for the next reaction to take place, by generating numbers $r \in (0,1)$ and setting $\tau = -n^{-1}\ln r$. After the waiting time, τ is generated, and the reaction is executed, hence the number of particles is updated, as is the time elapsed since the start of the dynamics. Reactions are executed one after the other at the right waiting time until all particles have decayed.

d. One must have $P_n(t)\,\mathrm{d}\,n = q(x,t)\,\mathrm{d}\,x$ where $n = Vx$ so $\frac{\mathrm{d}\,n}{\mathrm{d}\,x} = V$ and $q(x,t) = VP_n(t)$. Multiplying the master equation for $P_n(t)$ times V, and setting $n \pm 1 = V(x \pm {}^1\!/\!_V)$ and $VP_{n\pm1}(t) = q(x \pm V^{-1}, t)$ we have $\partial_t q(x,t) = -Vxq(x,t) + V(x + {}^1\!/\!_V)q(x + {}^1\!/\!_V, t)$. Taylor expanding

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

and inserting in the master equation for $q(x,t)$, the leading orders cancel and we are left with

$$\partial_t q(x,t) = \sum_{n=1}^{\infty} V^{1-n}\frac{\partial^n}{\partial x^n}[xq(x,t)]$$

Truncating to $n=2$ leads to the Fokker-Planck equation

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

e. Multiplying the master equation for $q(x,t)$ times x, integrating over x, solving the integrals by parts and setting the boundary terms to zero (due to probability and probability flux vanishing at the boundaries) we get

$$\partial_t \mathbb{E}[\mathsf{X}_t] = -\mathbb{E}[\mathsf{X}_t] \Rightarrow \mathbb{E}[\mathsf{X}_t] = \frac{N}{V}\,\mathrm{e}^{-t}\,.$$

Multiplying the master equation for $q(x,t)$ times x^2, integrating over x, solving the integrals by parts and setting the boundary terms to zero (due to probability and probability flux vanishing at the boundaries) we get

$$\partial_t \mathbb{E}[\mathsf{X}_t^2] = -2\mathbb{E}[\mathsf{X}_t^2] + \frac{1}{V}\mathbb{E}[\mathsf{X}_t] \Rightarrow \partial_t \mathbb{E}[\mathsf{X}_t^2] + 2\mathbb{E}[\mathsf{X}_t^2] = \frac{N}{V^2}\,\mathrm{e}^{-t}\,.$$

Using $\mathbb{E}[\mathsf{X}_0^2] = (N/V)^2$ as the initial condition is deterministic,

$$\mathbb{E}[\mathsf{X}_t^2] = \left(\frac{N}{V}\right)^2 \mathrm{e}^{-2t} + \frac{N}{V^2}(\mathrm{e}^{-t} - \mathrm{e}^{-2t}).$$

Problem 10.3

Absorbing boundary conditions in 0 and L means

$$p(0,t) = p(L,t) = 0 \quad \forall\ t.$$

We start writing the PDE in terms of the differential operator $\mathcal{W}$

$$\frac{\partial p(x,t)}{\partial t} = \mathcal{W} p(x,t).$$

Since $\mathcal{W}$ is Hermitian, it will have a complete set of orthonormal eigenfunctions

$$\mathcal{W}\psi_n(x) = \lambda_n \psi_n(x)$$

and one can expand $p(x,t)$ in terms of them

$$p(x,t) = \sum_n \alpha_n(t)\psi_n(x).$$

where $\alpha_n(t)$ is the inner product between $p(x,t)$ and $\psi_n(x)$

$$\alpha_n(t) = \int_0^L \mathrm{d}\, x\, \psi_n(x) p(x,t).$$

The eigenfunctions are found by solving the second-order ODE

$$D\frac{\partial^2}{\partial x^2}\psi_n(x) = \lambda_n \psi_n(x).$$

Giving the eigenvalues the usual order $\lambda_0 \geq \lambda_1 \geq \ldots \geq \lambda_L$, with $\lambda_0 = 0$ corresponding to the steady-state $\psi_0(x)$ and anticipating that $\lambda_n < 0\ \forall\ n > 0$, one has

$$\psi_n(x) = c_n \sin\left(\sqrt{\frac{|\lambda_n|}{D}}x\right) + c'_n \cos\left(\sqrt{\frac{|\lambda_n|}{D}}x\right)$$

Imposing the boundary conditions $\psi_n(0) = \psi_n(L) = 0$ gives $c'_n = 0$ and

$$\sqrt{\frac{|\lambda_n|}{D}} = \frac{n\pi}{L}$$

. Hence

$$\psi_n(x) = c_n \sin\left(\frac{n\pi x}{L}\right)$$

where c_n is found by imposing $\int \mathrm{d}\, x\, \psi_n(x)\psi_m(x) = \delta_{nm}$ and using the orthogonality relations:

$$\frac{1}{L}\int_{-L}^{L} \mathrm{d}\, x\, \sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right) = \begin{cases} 1 & n = m \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

giving $c_n^2 = {}^2/_L$. For $n = 0$ one has $\psi_0(x) = 0$, as obtained by directly solving the ODE for $\lambda_0 = 0$ and imposing the boundary conditions. It is easy to see that our boundary conditions cannot be satisfied by positive values of λ_n (which would lead to eigenfunctions which are exponential functions, rather than sin and cos). We can now integrate the equation for $p(x,t)$ using the found expansion,

$$p(x,t) = \mathrm{e}^{\mathcal{W}t}\, p(x,0) = \sum_n \alpha_n(0)\, \mathrm{e}^{\mathcal{W}t}\, \psi_n(x) = \sum_n \mathrm{e}^{\lambda_n t}\, \psi_n(x) \int_0^L \mathrm{d}\, x\, \psi_n(x) p(x,0)$$

$$= \frac{2}{L} \sum_{n=1}^{L} \mathrm{e}^{\lambda_n t} \sin\left(\frac{n\pi x}{L}\right) \int_0^L \mathrm{d}\, x\, \sin\left(\frac{n\pi x}{L}\right) p(x,0).$$

Note that $p(x,t)$ vanishes in the limit $t \to \infty$, due to the leaking through the boundaries. If fact, for absorbing boundary conditions, there is a non-zero probability current through the boundaries

$$J = -D \frac{\partial p(x,t)}{\partial x}.$$