

Chapter 2

Markovian Stochastic Processes

We elementarily review the mathematical theory of stochastic processes in this chapter. The main focus here is the correspondence between the stochastic differential equation (SDE) and the master equation (ME). The ME describes the time evolution of the probability distribution function (PDF), while the SDE describes the time evolution of stochastic quantities at the level of individual realizations [1, 2]. Although both approaches are equivalent [3, 4], the ME approach is useful for analytical calculations of PDFs for various systems. The SDE approach, which is useful for single trajectory analysis in particular, will be reviewed in Chap. 5 in detail.

For simplicity, we consider systems with a single-state variable in this chapter, though our method can be straightforwardly generalized for systems with multi-variables. For more technical details, see the textbooks by C.W. Gardiner, N.G. van Kampen, H. Risken, and H. Haken [1, 2, 5, 6]. For more rigorous formulations, see also the textbook by D. Applebaum [7].

We here remark our notation in this thesis. Variables with the hat symbol mean stochastic variables, such as \hat{A} ; bold Italic variables mean vectors, such as $\mathbf{A} \equiv (A_1, \dots, A_N)$; bold Italic variables with the hat symbol mean stochastic vectors, such as $\hat{\mathbf{A}} \equiv (\hat{A}_1, \dots, \hat{A}_N)$.

2.1 Master Equations

The Markov process is defined as the stochastic process whose time evolution for an infinitesimal time step dt depends only on the current state of the system, but does not depend on its past history. If a stochastic variable $\hat{v}(t)$ obeys the Markovian dynamics, in other words, its PDF $P(\hat{v}(t) = v) \equiv P_t(v)$ can be written as

$$\frac{\partial}{\partial t} P_t(v) = L P_t(v), \quad (2.1)$$

where L is a linear operator independent of time. Equation (2.1) is called the master equation (ME) or the differential form of the Chapman–Kolmogorov equation [1]. We next derive several concrete MEs from stochastic dynamics of $\hat{v}(t)$ to understand intuitive pictures of stochastic processes.

2.2 Ordinary Differential Equation Without Jumps

First of all, we consider the first-order deterministic ordinary differential equation

$$\frac{d\hat{v}}{dt} = -a(\hat{v}), \quad (2.2)$$

where $a(\hat{v})$ is an arbitrary smooth function. We assume that the initial distribution is given by $P(\hat{v}(0) = v_0) = P_0(v_0)$. Note that all of the stochastic properties are included in the initial distribution $P_0(v_0)$ in this case. The dynamics of this model is obviously independent of its history, and is thus Markovian. The corresponding ME is given by the Liouville equation as

$$\frac{\partial}{\partial t} P_t(v) = \frac{\partial}{\partial v} a(v) P_t(v) = -\frac{\partial}{\partial v} J_t(v) \quad (2.3)$$

with the probability current $J_t(v) \equiv -a(v)P_t(v)$, which implies the probability conservation.

Derivation: The derivation of Eq. (2.3) is as follows: let us consider an arbitrary smooth function $f(v)$. The time derivative of $f(\hat{v})$ is given by

$$\frac{df(\hat{v})}{dt} = \frac{df(\hat{v})}{d\hat{v}} \frac{d\hat{v}}{dt} = -\frac{df(\hat{v})}{d\hat{v}} a(\hat{v}). \quad (2.4)$$

By taking the ensemble averages $\langle \cdots \rangle$ of both hand sides, we obtain the following identity

$$\begin{aligned} \left\langle \frac{df(\hat{v})}{dt} \right\rangle &= \left\langle -\frac{df(\hat{v})}{d\hat{v}} a(\hat{v}) \right\rangle \\ \frac{d}{dt} \int_{-\infty}^{\infty} dv f(v) P_t(v) &= - \int_{-\infty}^{\infty} dv P_t(v) a(v) \frac{df(v)}{dv} \\ \int_{-\infty}^{\infty} dv f(v) \frac{\partial P_t(v)}{\partial t} &= \int_{-\infty}^{\infty} dv f(v) \frac{\partial}{\partial v} [a(v) P_t(v)], \end{aligned} \quad (2.5)$$

where we have used the exchange of the limitations $\langle df(\hat{v})/dt \rangle = d\langle f(\hat{v}) \rangle/dt$ and the partial integration. Because this identity holds for an arbitrary function $f(v)$, Eq. (2.3) is then derived.¹

2.3 Ordinary Differential Equation with Jumps

We next consider a dynamical equation driven by a deterministic impulse at $t = \tau_c$ (Fig. 2.1a, b)

$$\frac{d\hat{v}}{dt} = -a(\hat{v}) + F^{\text{ext}}, \quad F^{\text{ext}} = y^* \delta(t - \tau_c), \quad (2.6)$$

where $a(\hat{v})$ is a smooth function and y^* is the velocity jump. The initial position is assumed to distribute according to $P(\hat{v}(0) = v_0) = P_0(v_0)$. This type dynamics appears for systems with a deterministic particle collision, where the jump size y^* is determined by classical mechanics (Fig. 2.1c). The time evolution of the PDF obeys a pseudo-Liouville equation

$$\frac{\partial}{\partial t} P_t(v) = \frac{\partial}{\partial v} a(v) P_t(v) + [P_t(v - y^*) - P_t(v)] \delta(t - \tau_c). \quad (2.7)$$

This is the master equation for Eq. (2.6) and is nonlocal in terms of velocity. The nonlocal property originates from the δ -impulse inducing a finite jump of the trajectory.

Derivation: The pseudo-Liouville equation (2.7) is derived as follows. Let us consider an arbitrary smooth function $f(v)$ and its time evolution during an infinitesimal time interval dt .

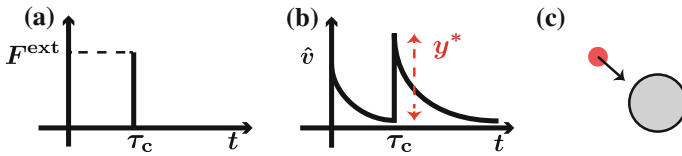


Fig. 2.1 **a** Deterministic impulse $F^{\text{ext}}(t) = y^* \delta(t - \tau_c)$. **b** Dynamics of Eq. (2.6), driven by the impulse with $a(\hat{v}) = \hat{v}$. **c** Particle collision at the time τ_c as a physical example

¹Let us consider two smooth functions $f(x)$ and $g(x)$. If an identity $h(x) \int_{-\infty}^{\infty} dx f(x) h(x) = \int_{-\infty}^{\infty} dx g(x) h(x)$ for an arbitrary smooth function $h(x)$, $f(x)$ and $g(x)$ are identical. This identity can be shown by substituting $h(x)$ by $f(x) - g(x)$. We indeed obtain $\int_{-\infty}^{\infty} dx \{f(x) - g(x)\}^2 = 0$, which implies $f(x) = g(x)$.

$$df(\hat{v}(t)) \equiv f(\hat{v}(t+dt)) - f(\hat{v}(t)) = \begin{cases} -a(\hat{v}) \frac{df(\hat{v}(t))}{d\hat{v}} dt & (\tau_c \notin [t, t+dt]) \\ f(\hat{v}(t) + y^*) - f(\hat{v}(t)) & (\tau_c \in [t, t+dt]) \end{cases} \quad (2.8)$$

up to leading order. This relation can be rewritten as

$$\frac{df(\hat{v}(t))}{dt} = -a(\hat{v}) \frac{df(\hat{v}(t))}{d\hat{v}} + [f(\hat{v}(t) + y^*) - f(\hat{v}(t))] \delta(t - \tau_c), \quad (2.9)$$

where the multiplication between $f(\hat{v}(t) + y^*) - f(\hat{v}(t))$ and $\delta(t - \tau_c)$ is the forward Euler type in terms of time as $[f(\hat{v}(t) + y^*) - f(\hat{v}(t))] \delta(t - \tau_c) = [f(\hat{v}(\tau_c - 0) + y^*) - f(\hat{v}(\tau_c - 0))] \delta(t - \tau_c)$. This multiplication is implicitly the Itô product, which will be studied in detail in Chaps. 5 and 9. We use this convention for δ -functions in this chapter. By taking the ensemble averages of both hand side, we obtain

$$\begin{aligned} \left\langle \frac{df(\hat{v}(t))}{dt} \right\rangle &= \left\langle -a(\hat{v}(t)) \frac{df(\hat{v}(t))}{d\hat{v}} + [f(\hat{v}(t) + y^*) - f(\hat{v}(t))] \delta(t - \tau_c) \right\rangle \\ \int_{-\infty}^{\infty} dv f(v) \frac{\partial P_t(v)}{\partial t} &= \int_{-\infty}^{\infty} dv \left\{ -a(v) \frac{df(v)}{dv} + [f(v + y^*) - f(v)] \delta(t - \tau_c) \right\} P_t(v) \\ \int_{-\infty}^{\infty} dv f(v) \frac{\partial P_t(v)}{\partial t} &= \int_{-\infty}^{\infty} dv \left\{ \frac{\partial}{\partial v} a(v) P_t(v) + [P_t(v - y^*) - P_t(v)] \delta(t - \tau_c) \right\} f(v). \end{aligned} \quad (2.10)$$

Equation (2.7) is then derived since this identity holds for an arbitrary function $f(v)$. This technique is frequently used for the derivation of various MEs and is summarized in Fig. 2.2.

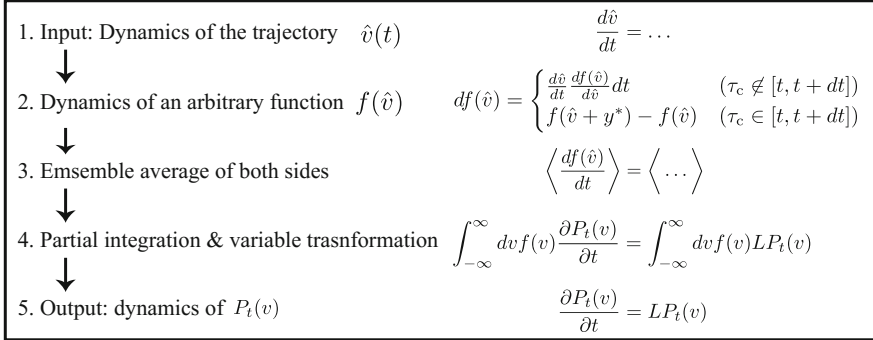


Fig. 2.2 Conceptual diagram for the derivation of MEs from SDEs, where τ_c is a jump time. Case analysis is necessary in the presence of trajectory jumps. This procedure is frequently followed to derive various MEs throughout this thesis

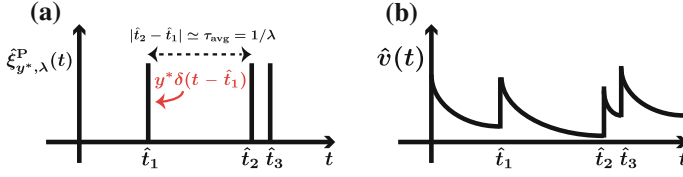


Fig. 2.3 **a** A typical trajectory of the Poisson noise. **b** A typical trajectory of a system driven by the Poisson noise in the case $a(\hat{v}) = \hat{v}$

2.4 Poisson Noise

We next define the white Poisson noise as the most basic element of the Markovian stochastic processes. The white Poisson noise represents a sequence of microscopic discrete events such as random particle collisions, and is described by the δ -function type impulses. The Poisson noise is characterized by the transition rate² λ and the jump distance y^* . The transition rate λ characterizes the frequency of random events: the probability of a Poisson jump during $[t, t + dt]$ is given by λdt . Let us consider the time series of the Poisson jumps as $\{\hat{t}_i\}_{i \geq 1}$, which is generated by the above stochastic rule and uniquely determines the trajectory of the Poisson noise. Note that the time interval between two successive jumps $\Delta \hat{t}_i \equiv \hat{t}_{i+1} - \hat{t}_i$ obeys the exponential distribution³ $P(\Delta \hat{t}_i) = \lambda e^{-\lambda \Delta \hat{t}_i}$, and the average time interval is given by $\tau_{\text{avg}} \equiv \langle |\hat{t}_{i+1} - \hat{t}_i| \rangle = 1/\lambda$. The explicit form of the Poisson noise can be written as

$$\hat{\xi}_{y^*, \lambda}^{\text{P}}(t) = \sum_{i=1}^{\infty} y^* \delta(t - \hat{t}_i). \quad (2.11)$$

As seen from Fig. 2.3a, the trajectory of the Poisson noise is singular because of the δ -functions, which is a mathematically important issue. We next consider a stochastic process driven by a Poisson noise

$$\frac{d\hat{v}}{dt} = -a(\hat{v}) + \hat{\xi}_{y^*, \lambda}^{\text{P}}(t), \quad (2.12)$$

where $a(\hat{v})$ is an arbitrary smooth function. A typical trajectory of the system driven by the Poisson noise is given in Fig. 2.3b for the case $a(\hat{v}) = \hat{v}$, where finite jumps of the trajectory exists because of the δ -type singularity of the Poisson noise. The corresponding ME is given by

²The transition rate is also known as intensity or collision rate [1].

³The derivation is as follows: the probability where the interval $\Delta \hat{t}_i$ is not shorter than t is denoted by $P(\Delta \hat{t}_i \geq t) \equiv \int_t^{\infty} d(\Delta \hat{t}_i) P(\Delta \hat{t}_i)$. $P(\Delta \hat{t}_i \geq t)$ satisfies $P(\Delta \hat{t}_i \geq t + dt) = (1 - \lambda dt) P(\Delta \hat{t}_i \geq t) \iff dP(\Delta \hat{t}_i \geq t)/dt = -\lambda P(\Delta \hat{t}_i \geq t)$. We thus obtain $P(\Delta \hat{t}_i \geq t) = e^{-\lambda t} \implies P(\Delta \hat{t}_i) = -(dP(\Delta \hat{t}_i \geq t)/dt)|_{t=\Delta \hat{t}_i} = \lambda e^{-\lambda \Delta \hat{t}_i}$.

$$\frac{\partial P_t(v)}{\partial t} = \frac{\partial}{\partial v} a(v) P_t(v) + \lambda [P_t(v - y^*) - P_t(v)], \quad (2.13)$$

where the terms $(\partial/\partial v)[a(v)P_t(v)]$, $\lambda P_t(v - y^*)$, and $-\lambda P_t(v)$ imply the deterministic evolution, the probability inflow to v , and the probability outflow from v , respectively. The ME (2.13) is nonlocal in terms of velocity because of the Poisson jumps. The Poisson noise can be simply rewritten as

$$\hat{\xi}_{y^*,\lambda}^P(t) = y^* \hat{\xi}_\lambda^P(t), \quad (2.14)$$

where $\hat{\xi}_\lambda^P(t) \equiv \hat{\xi}_{y^*=1,\lambda}^P(t)$ is the standard Poisson noise with unit jump size $y^* = 1$.

Derivation: Let us consider an arbitrary smooth function $f(v)$ and its dynamics for an infinitesimal time interval $[t, t + dt]$

$$df(\hat{v}(t)) \equiv f(\hat{v}(t + dt)) - f(\hat{v}(t)) = \begin{cases} -a(\hat{v}) \frac{df(\hat{v}(t))}{d\hat{v}} dt & (\hat{t}_i \in [t, t + dt] : \text{Prob.} = 1 - \lambda dt) \\ f(\hat{v}(t) + y^*) - f(\hat{v}(t)) & (\hat{t}_i \notin [t, t + dt] : \text{Prob.} = \lambda dt) \end{cases} \quad (2.15)$$

up to leading order. By taking the ensemble averages of both hand sides, we obtain

$$\begin{aligned} \left\langle f(\hat{v}(t + dt)) - f(\hat{v}(t)) \right\rangle &= (1 - \lambda dt) \left\langle -a(\hat{v}(t)) \frac{df(\hat{v}(t))}{d\hat{v}} dt \right\rangle + \lambda dt \left\langle [f(\hat{v}(t) + y^*) - f(\hat{v}(t))] \right\rangle \\ \int_{-\infty}^{\infty} dv f(v) [P_{t+dt}(v) - P_t(v)] &= \int_{-\infty}^{\infty} dv \left\{ -a(v) \frac{df(v)}{dv} dt + \lambda [f(v + y^*) - f(v)] dt \right\} P_t(v) + O(dt^2) \\ \int_{-\infty}^{\infty} dv f(v) \frac{\partial}{\partial t} P_t(v) dt &= \int_{-\infty}^{\infty} dv \left\{ \frac{\partial}{\partial v} a(v) P_t(v) + \lambda [P_t(v - y^*) - P_t(v)] \right\} f(v) dt + O(dt^2), \end{aligned} \quad (2.16)$$

which implies

$$\int_{-\infty}^{\infty} dv f(v) \frac{\partial}{\partial t} P_t(v) = \int_{-\infty}^{\infty} dv \left\{ \frac{\partial}{\partial v} a(v) P_t(v) + \lambda [P_t(v - y^*) - P_t(v)] \right\} f(v). \quad (2.17)$$

This identity holds for an arbitrary smooth $f(v)$, and the ME (2.13) is then derived.

Differential form: We next see the singularity of the trajectory in the differential form. We note that the following differential form is useful in the later discussion on the Gaussian noise. Let us define the Poisson process as $d\hat{N}_{y^*,\lambda}^P/dt = \hat{\xi}_{y^*,\lambda}^P \iff \hat{N}_{y^*,\lambda}^P(t) = \int_0^t dt' \hat{\xi}_{y^*,\lambda}^P(t')$. During an infinitesimal interval $[t, t + dt]$, $d\hat{N}_{y^*,\lambda}^P(t) \equiv \hat{N}_{y^*,\lambda}^P(t + dt) - \hat{N}_{y^*,\lambda}^P(t)$ takes the following values:

$$d\hat{N}_{y^*,\lambda}^P = \begin{cases} y^* & (\hat{t}_i \in [t, t + dt] : \text{Prob.} = \lambda dt) \\ 0 & (\hat{t}_i \notin [t, t + dt] : \text{Prob.} = 1 - \lambda dt) \end{cases}, \quad (2.18)$$

or

$$\left(d\hat{N}_{y^*,\lambda}^P\right)^n = \begin{cases} y^{*n} & (\hat{t}_i \in [t, t + dt] : \text{Prob.} = \lambda dt) \\ 0 & (\hat{t}_i \notin [t, t + dt] : \text{Prob.} = 1 - \lambda dt) \end{cases} \quad (2.19)$$

for some integer i . We then obtain the moments

$$\left\langle \left(d\hat{N}_{y^*,\lambda}^P\right)^n \right\rangle = \lambda y^{*n} dt. \quad (2.20)$$

Remarkably, all the moments are the same order of $O(dt)$ because of jumps along the trajectories, which implies that all moments are relevant even for the differential forms.

2.4.1 Symmetric Poisson Noise

The Poisson noise is the basic element of the Markovian stochastic processes, and various noises can be composed of the Poisson noise. In the following, we discuss several noises composed of the Poisson noise. We first study the symmetric Poisson noise defined by

$$\hat{\xi}_{y^*,\lambda}^{\text{SP}}(t) \equiv \hat{\xi}_{y^*,\lambda/2}^P(t) + \hat{\xi}_{-y^*,\lambda/2}^P(t), \quad (2.21)$$

where $\hat{\xi}_{y^*,\lambda/2}^P(t)$ and $\hat{\xi}_{-y^*,\lambda/2}^P(t)$ are independent. A typical trajectory of the symmetric Poisson is illustrated in Fig. 2.4a. We also consider a system drive by the symmetric Poisson noise as

$$\frac{d\hat{v}}{dt} = -a(\hat{v}) + \hat{\xi}_{y^*,\lambda}^{\text{SP}}(t). \quad (2.22)$$

A typical trajectory of the system is illustrated in Fig. 2.4b for the case $a(\hat{v}) = \hat{v}$. The master equation of Eq. (2.22) is given by

$$\frac{\partial P_t(v)}{\partial t} = \frac{\partial}{\partial v} a(v) P_t(v) + \frac{\lambda}{2} [P_t(v - y^*) - P_t(v)] + \frac{\lambda}{2} [P_t(v + y^*) - P_t(v)], \quad (2.23)$$

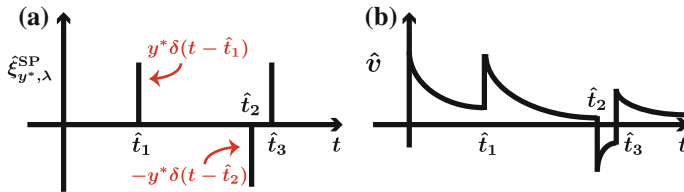


Fig. 2.4 **a** A typical trajectory of the symmetric Poisson noise. **b** A typical trajectory of a system driven by the symmetric Poisson noise for $a(\hat{v}) = \hat{v}$

where the first term on the right-hand side originates from $-a(\hat{v})$, the second term originates from $\hat{\xi}_{y^*, \lambda/2}^P$, and the third term originates from $\hat{\xi}_{-y^*, \lambda/2}^P$. The ME (2.23) is nonlocal in terms of velocity because of jumps of a trajectory induced by the symmetric Poisson noise.

Differential form: We here note the differential form for the symmetric Poisson process defined by $d\hat{N}_{y^*, \lambda}^{\text{SP}}/dt = \hat{\xi}_{y^*, \lambda}^{\text{SP}} \iff \hat{N}_{y^*, \lambda}^{\text{SP}}(t) = \int_0^t dt' \hat{\xi}_{y^*, \lambda}^{\text{SP}}(t')$. The moments of the differential form $d\hat{N}_{y^*, \lambda}^{\text{SP}}$ are given by

$$\langle (d\hat{N}_{y^*, \lambda}^{\text{SP}})^n \rangle = \begin{cases} 0 & (\text{odd } n) \\ \lambda y^{*n} dt & (\text{even } n) \end{cases}. \quad (2.24)$$

2.4.2 Discrete Compound Poisson Noise

The symmetric Poisson noise is composed of two independent Poisson noises. As a straightforward generalization, the discrete compound Poisson noise is constructed as a combination of the Poisson noises (Fig. 2.5a) as

$$\hat{\xi}_{y^*, \lambda}^{\text{CP}}(t) \equiv \sum_{k=1}^{N_{\text{CP}}} \hat{\xi}_{y_k^*, \lambda_k}^P(t) = \sum_{k=1}^{N_{\text{CP}}} y_k^* \hat{\xi}_{\lambda_k}^P(t) \quad (2.25)$$

for velocity jump sizes $y^* \equiv (y_1^*, \dots, y_{N_{\text{CP}}}^*)$ and transition rates $\lambda \equiv (\lambda_1, \dots, \lambda_{N_{\text{CP}}})$. N_{CP} can be infinity and the Poisson noise terms $\hat{\xi}_{y_k^*, \lambda_k}^P(t)$ are independent of each other. Let us consider a system driven by the compound Poisson noise (2.25) as

$$\frac{d\hat{v}}{dt} = -a(\hat{v}) + \hat{\xi}_{y^*, \lambda}^{\text{CP}}, \quad (2.26)$$

where $a(\hat{v})$ is an arbitrary smooth function. The ME for Eq. (2.26) is given similarly to Eq. (2.23):

$$\frac{\partial P_t(v)}{\partial t} = \frac{\partial}{\partial v} a(v) P_t(v) + \sum_{k=1}^{N_{\text{CP}}} \lambda_k [P_t(v - y_k^*) - P_t(v)]. \quad (2.27)$$

The symmetric Poisson noise is a special discrete compound Poisson noise with velocity jump sizes $y^* = (+y^*, -y^*)$, transition rates $\lambda = (\lambda/2, \lambda/2)$, and $N_{\text{CP}} = 2$. We also note that the ME (2.27) is a nonlocal equation in terms of velocity because of Poisson jumps.

2.4.3 Continuous Compound Poisson Noise

The discrete compound Poisson process can be generalized for the continuous compound Poisson noise (see Fig. 2.5b for a schematic). Let us introduce the transition rate density $\lambda(y)$ with jump distance y : the probability where a Poisson jump happens with jump size $y^* \in [y, y + dy]$ during a time interval $[t, t + dt]$ is given by

$$\lambda(y)dydt. \quad (2.28)$$

In the following, the transition rate density is called the transition rate for short. We then define the compound Poisson process with transition rate $\lambda(y)$ as

$$\hat{\xi}_{\lambda(y)}^{\text{CP}}(t) \equiv \int_y \hat{\xi}_{y, dy\lambda(y)}^{\text{P}}(t) = \int_y y \hat{\xi}_{dy\lambda(y)}^{\text{P}}(t), \quad (2.29)$$

where \int_y formally represents the continuous summation for $y \in (-\infty, \infty)$ [7]. The average interval between two successive jumps $\tau_{\text{avg}} \equiv \langle |t_{i+1} - t_i| \rangle$ is given by $1/\tau_{\text{avg}} = \int dy \lambda(y)$, and jump size obeys the distribution $P(y) = \lambda(y) / \int dy \lambda(y)$. We note that the continuous compound Poisson noise reduces to the ordinary Poisson noise for $\lambda(y) = \lambda^* \delta(y - y^*)$ as $\hat{\xi}_{\lambda(y)}^{\text{CP}} = \int_y \hat{\xi}_{y, dy\lambda(y)}^{\text{P}} = \hat{\xi}_{y^*, \lambda^*}^{\text{P}}$.

Here we consider the following system driven by the compound Poisson noise as

$$\frac{d\hat{v}}{dt} = -a(\hat{v}) + \hat{\xi}_{\lambda(y)}^{\text{CP}}(t). \quad (2.30)$$

The corresponding ME is given by

$$\frac{\partial P_t(v)}{\partial t} = \frac{\partial}{\partial v} a(v) P_t(v) + \int_{-\infty}^{\infty} dy \lambda(y) [P_t(v - y) - P_t(v)], \quad (2.31)$$

which is an integro-differential equation, spatially nonlocal because of the Poisson jumps.

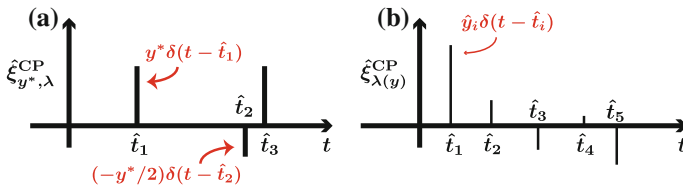


Fig. 2.5 **a** Schematic trajectory of the discrete compound Poisson noise with $N = 2$, $y^* = (y^*, -y^*/2)$, and $\lambda = (\lambda/2, \lambda/2)$. **b** Schematic trajectory of the continuous compound Poisson noise. As an example, the two-sided exponential Poisson noise is illustrated for $\lambda(y) = e^{-|y|/y^*}/2\tau^*y^*$ with typical jump size y^* and average time interval τ^*

2.5 Gaussian Noise

The Poisson noise is a strongly singular noise causing jumps along a trajectory. We next consider a stochastic process where jumps of trajectory are infinitesimal: let us take the small jump limit $y^* \rightarrow 0$ for the symmetric Poisson noise $\hat{\xi}_{y^*,\lambda}^{\text{SP}}$ with the variance kept constant $\sigma^2 \equiv \lambda y^{*2} = \text{const.}$ (see Fig. 2.6a, c for schematics) as

$$\hat{\xi}_{\sigma^2}^{\text{G}}(t) \equiv \lim_{y^* \rightarrow 0} \hat{\xi}_{y^*,\lambda}^{\text{SP}}(t). \quad (2.32)$$

The noise defined in Eq. (2.32) is called the Gaussian noise. In particular, we denote the Gaussian noise with unit variance by $\hat{\xi}^{\text{G}}(t) \equiv \hat{\xi}_{\sigma^2=1}^{\text{G}}(t)$. In this limit, jump size by the noise is infinitesimal (i.e., $y^* \rightarrow 0$) whereas noise happens frequently (i.e., $\lambda \rightarrow \infty$).

Let us consider a system driven by the Gaussian noise next

$$\frac{d\hat{v}}{dt} = -a(\hat{v}) + \hat{\xi}_{\sigma^2}^{\text{G}}(t), \quad (2.33)$$

where $a(\hat{v})$ is an arbitrary smooth function. A typical trajectory of the system (2.33) is illustrated in Fig. 2.6d, which is obtained in the Gaussian limit from the symmetric Poisson noise in Fig. 2.6a, b. The ME for Eq. (2.33) is the Fokker–Planck equation

$$\frac{\partial P_t(v)}{\partial t} = \left[\frac{\partial}{\partial v} a(v) + \frac{\sigma^2}{2} \frac{\partial^2}{\partial v^2} \right] P_t(v). \quad (2.34)$$

Remarkably, the Fokker–Planck equation (2.34) belongs to the class of the local partial differential equations in terms of velocity, which are crucially different from the MEs for the Poisson noises.

Derivation: The derivation of Eq. (2.23) is below. Let us apply the Taylor expansion to the ME (2.23) for the symmetric Poisson noise as

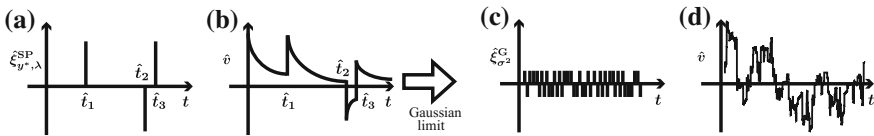


Fig. 2.6 **a, b** Typical trajectories of the symmetric Poisson noise and the system driven by the noise for $a(\hat{v}) = \hat{v}$. **c, d** Gaussian limit from the symmetric Poisson noise ($y^* \rightarrow 0$, $\lambda y^{*2} = \sigma^2 = \text{const.}$). A typical trajectory of the Gaussian noise is illustrated in the figure (c), and a typical trajectory of the system driven by the Gaussian noise is illustrated in the figure (d)

$$\begin{aligned}
\frac{\partial P_t(v)}{\partial t} &= \frac{\partial}{\partial v} a(v) P_t(v) + \frac{\lambda}{2} [P_t(v - y^*) + P_t(v + y^*) - 2P_t(v)] \\
&= \frac{\partial}{\partial v} a(v) P_t(v) + \sum_{n=1}^{\infty} \frac{\lambda y^{*2n}}{(2n)!} \frac{\partial^{2n}}{\partial v^{2n}} P_t(v).
\end{aligned} \tag{2.35}$$

The ME (2.23) is derived by taking the Gaussian limit $y^* \rightarrow 0$ with $\lambda y^{*2} = \sigma^2 = \text{const.}$

Differential form: We here note a unique character of the differential form of the Gaussian noise. Let us consider the following stochastic quantity:

$$\hat{W}(t) \equiv \int_0^t ds \hat{\xi}^G(s) \iff d\hat{W} = \hat{\xi}^G dt, \tag{2.36}$$

where \hat{W} is called the Wiener process. We note that the Gaussian noise is formally defined as the difference of the Wiener process mathematically. The Wiener process has a unique property in terms of differential forms. All of the moments over the third-order are zero as

$$\langle (d\hat{W})^n \rangle = \begin{cases} dt & (n = 2) \\ 0 & (\text{otherwise}) \end{cases}. \tag{2.37}$$

This property will be utilized as the Itô rule, as will be shown in Chap 5.

2.6 White Noise

We study the white noise in this section. White noise is the noise which does not have time correlation and environmental correlation with the state of the system \hat{v} . In other words, if $\hat{\xi}^W$ is the white noise, the following relation holds for an arbitrary time t_1, t_2 , and $t_3 \leq \min\{t_1, t_2\}$:

$$\left\langle \left[\hat{\xi}^W(t_1) - \langle \hat{\xi}^W(t_1) \rangle \right] \left[\hat{\xi}^W(t_2) - \langle \hat{\xi}^W(t_2) \rangle \right] \right\rangle_{\hat{v}(t_3)=v} = C \delta(t_1 - t_2), \tag{2.38}$$

where $\langle \cdots \rangle_{\hat{v}(t)=v}$ is the ensemble average on the condition $\hat{v}(t) = v$ and C is a constant independent of t_1, t_2, t_3 , and v . The Lévy-Itô decomposition [1, 8] states that any white noise $\hat{\xi}^W$ can be decomposed into the constant drift, the Gaussian noise, and the compound Poisson noise⁴

$$\hat{\xi}^W(t) = m + \hat{\xi}_{\sigma^2}^G(t) + \hat{\xi}_{\lambda(y)}^{\text{CP}}(t) = m + \sigma \hat{\xi}^G(t) + \int_y \hat{\xi}_{y, dy \lambda(y)}^{\text{P}}(t), \tag{2.39}$$

⁴Here, the transition rate is assumed not singular and the total transition rate is finite as $\int dy \lambda(y) < \infty$.

with a real number (constant drift) m , a nonnegative real number (variance) $\sigma^2 \geq 0$, and a nonnegative real function (transition rate) $\lambda(y) \geq 0$. This theorem guarantees that any non-Gaussian white noise is composed of the Poisson noises. Furthermore, the Gaussian noise is also obtained as the limit of the symmetric Poisson noise as shown in Sect. 2.5, which implies that the Poisson noise is the basic component of any white noise. The ME of a system drive by a general white noise $\hat{\xi}^W$ is given by

$$\frac{\partial P_t(v)}{\partial t} = \left[\frac{\partial}{\partial v} \{a(v) - m\} + \frac{\sigma^2}{2} \frac{\partial^2}{\partial v^2} \right] P_t(v) + \int_{-\infty}^{\infty} dy \lambda(y) [P_t(v - y) - P_t(v)], \quad (2.40)$$

where the stochastic dynamics of the systems is described by

$$\frac{d\hat{v}}{dt} = -a(\hat{v}) + \hat{\xi}^W \quad (2.41)$$

with a smooth function $a(\hat{v})$.

Lévy process: We here remark that the white noise is defined as the formal derivative of the Lévy processes in mathematics. The Lévy process $\hat{L}(t)$ is defined as

$$\hat{L}(t) \equiv \int_0^t ds \hat{\xi}^W(s), \quad (2.42)$$

where $\hat{\xi}^W$ is the white noise. Because the integration in Eq. (2.42) removes the singularity of the white noise $\hat{\xi}^W$, the Lévy process \hat{L} has better properties than the white noise $\hat{\xi}^W$. In the context of mathematics, therefore, the Lévy process \hat{L} is a more central issue than the white noise $\hat{\xi}^W$.

2.7 General Master Equation

We have argued MEs for various white noises. General Markovian processes, however, are not driven only by white noise, but also by noise which has environmental correlation with the state of the system \hat{v} . In other words, the variance of the Gaussian noise σ^2 and the transition rate $\lambda(y)$ can depend on the state variable \hat{v} as $\sigma^2 \rightarrow \sigma^2(v)$ and $\lambda(y) \rightarrow \lambda(y; v)$. The most general form of the Markovian processes with a single variable \hat{v} is therefore given by the following form:

$$\frac{\partial P_t(v)}{\partial t} = \left[\frac{\partial}{\partial v} a(v) + \frac{1}{2} \frac{\partial^2}{\partial v^2} \sigma^2(v) \right] P_t(v) + \int_{-\infty}^{\infty} dy [\lambda(y; v - y) P_t(v - y) - \lambda(y; v) P_t(v)], \quad (2.43)$$

where $\sigma(v)$ and $\lambda(y; v)$ are the standard deviation of the Gaussian noise and the transition rate of the compound Poisson noise on the condition of $\hat{v}(t) = v$,

respectively.⁵ Because of the correlation between the noise and the system (i.e., $\sigma(\hat{v})$ and $\lambda(y; \hat{v})$ depend on \hat{v}), the SDE corresponding to the general ME (2.43) is not naively written as a system driven by white noise. The corresponding SDE is given as the system driven by state-dependent noises

$$\frac{d\hat{v}}{dt} = -a(\hat{v}) + \sigma(\hat{v}) \cdot \hat{\xi}^G + \hat{\xi}_{\lambda(y; \hat{v})}^{\text{CP}}, \quad (2.44)$$

where $\lambda(y; v)$ is the transition rate with jump distance y under the condition of $\hat{v}(t) = v$. We here note that the second and third terms on the right-hand side of Eq. (2.44) should be interpreted in the Itô sense (the forward Euler product),⁶ which will be discussed in Chaps. 5 and 9.

2.8 Kramers–Moyal Expansion

The ME (2.43) is an integro-differential equation. However, the ME can be rewritten into an infinite-order differential form, called the Kramers–Moyal (KM) expansion. Let us assume that $\lambda(y; v - y)P_t(v - y)$ is a sufficiently smooth function (e.g., a C^∞ -function), which implies that the following identity formally holds:

$$\int_{-\infty}^{\infty} dy \lambda(y; v - y) P_t(v - y) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{-\infty}^{\infty} dy y^n \frac{\partial^n}{\partial v^n} \lambda(y; v) P_t(v). \quad (2.45)$$

On the basis of this identity, we obtain

$$\frac{\partial P_t(v)}{\partial t} = \left[\frac{\partial}{\partial v} a(v) + \frac{1}{2} \frac{\partial^2}{\partial v^2} b^2(v) + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial v^n} \alpha_n(v) \right] P_t(v), \quad \alpha_n(v) \equiv \int_{-\infty}^{\infty} dy y^n \lambda(y; v) \quad (2.46)$$

where $\alpha_n(v)$ is the KM coefficient. If we truncate the KM expansion up to the second-order, the Fokker–Planck equation is reproduced. This expansion was historically recognized as a formal derivation of the Fokker–Planck equation, but was criticized by van Kampen because the validity of such truncation is unclear in the absence of explicit perturbative parameters [1]. Van Kampen finally revealed the explicit condition to validate the second-order truncation in Refs. [2, 9], as will be reviewed as the system size expansion in Chap. 4.

Pawula theorem: The KM coefficients are not independent of each other and arbitrary values cannot be substituted into them. The Pawula theorem highlights this property [5]: $\alpha_n(v) = 0$ for all $n \geq 3$, if $\alpha_{2k}(v) = 0$ for some $k \geq 1$. This implies that the truncation of the KM expansion is valid only up to the second-order mathematically. If we truncate the expansion up to higher order, solutions of MEs do not satisfy the nonnegativity of PDFs.

⁵The generality of Eq. (2.43) is proved in Ref. [1].

⁶The symbol “ \cdot ” implies the Itô product (the Itô integral).

We note that this theorem does not necessarily restrict from us the truncation of higher order terms for the purpose of perturbation [5]. When we apply the system size expansion (see Sect. 4.2), for example, we can formally obtain high-order perturbative solutions for MEs. Though the nonnegativity of PDFs is violated in such perturbative solutions, they may be useful for calculation of moments because negative probability may appear only in the tail of the PDF and does not necessarily contribute to the calculation of moments dominantly.

Failure of the KM expansion: The Kramers–Moyal expansion may sometimes fail when a system has singularities and its PDF is not a C^∞ -function correspondingly. In the presence of the Coulombic friction (see Sect. 8.3.4), for example, the PDF has a singular peak and is a piecewise smooth function. The Kramers–Moyal expansion fails for this model because of this singularity (see Appendix A.1.1 for details).

2.9 Cumulant Generating Function for the White Noise

We here note the explicit form of the cumulant generating function for the white noise $\hat{\xi}^W(t)$. The cumulant generating function $\Phi(s)$ is defined as

$$\Phi(s) = \frac{1}{t} \log \langle e^{is\hat{L}(t)} \rangle, \quad (2.47)$$

where we have introduced the Lévy process $\hat{L}(t) \equiv \int_0^t ds \hat{\xi}^W(s)$. The cumulant generating functions for the Gaussian noise $\hat{\xi}^G(t)$, the Poisson noise $\hat{\xi}_{y^*,\lambda}^P(t)$, and the continuous compound Poisson noise $\hat{\xi}_{\lambda(y)}^{CP}(t)$ are given by

$$\Phi_{\sigma^2}^G(s) = -\frac{\sigma^2}{2}s^2, \quad \Phi_{y^*,\lambda}^P(s) = \lambda(e^{isy^*} - 1), \quad \Phi_{\lambda(y)}^{CP}(s) = \int_{-\infty}^{\infty} dy \lambda(y)(e^{isy} - 1). \quad (2.48)$$

The cumulant generating function for the white noise can be represented by the Lévy-Khinchin formula [8] as

$$\Phi(s) = ism - \frac{\sigma^2 s^2}{2} + \int_{-\infty}^{\infty} dy \lambda(y)(e^{isy} - 1), \quad (2.49)$$

which is equivalent to the Lévy-Itô decomposition (2.39).

2.10 Cumulant Generating Functional

The cumulant generating function can be generalized for the cumulant generating functional, which is useful for calculation of multiple-time cumulants. In this thesis, squared brackets $[\dots]$ are accompanied by any functional, such as $f[\zeta(s); t]$ for an argument function $\{\zeta(s)\}_{0 \leq s \leq t}$. The cumulant generating functional for a stochastic variable \hat{v} is defined by

$$\begin{aligned} \Phi[\zeta(s); t] &\equiv \log \left\langle \exp \left(i \int_0^t ds \zeta(s) \hat{v}(s) \right) \right\rangle \\ &= \sum_{n=1}^{\infty} \int_0^t ds_1 \dots \int_0^t ds_n \frac{i^n}{n!} K_n(s_1, \dots, s_n) \zeta(s_1) \dots \zeta(s_n) \end{aligned} \quad (2.50)$$

where we have used a functional Taylor expansion with multiple-time cumulant [10]

$$K_n(s_1, \dots, s_n) \equiv \left. \frac{i^{-n} \delta^n \Phi[\zeta(s); t]}{\delta \zeta(s_1) \dots \delta \zeta(s_n)} \right|_{\zeta=0} = \langle v(s_1) \dots v(s_n) \rangle_c. \quad (2.51)$$

For white noise $\hat{\xi}^W$, the multiple-time cumulants are given by

$$K_n(s_1, \dots, s_n) = K_n \delta(s_1, \dots, s_n), \quad K_n = \sigma^2 \delta_{n,2} + \int_{-\infty}^{\infty} dy y^n \lambda(y) \quad (2.52)$$

with n -points δ -function $\delta(s_1, \dots, s_n)$ and the Kronecker delta $\delta_{n,m}$. Note that the n -points δ -function satisfies the following relation:

$$\delta_n(t_1, \dots, t_n) = \begin{cases} +\infty & (t_1 = \dots = t_n) \\ 0 & (\text{otherwise}) \end{cases}, \quad \int_{-\infty}^{+\infty} dt_2 \dots \int_{-\infty}^{+\infty} dt_n \delta_n(t_1, t_2, \dots, t_n) = 1. \quad (2.53)$$

Let us denote an arbitrary permutation of $\{t_i\}_{1 \leq n \leq n}$ by $\{s_i\}_{1 \leq i \leq n}$. By assuming a symmetry

$$\delta_n(t_1, \dots, t_n) = \delta_n(s_1, \dots, s_n), \quad (2.54)$$

we also obtain

$$\int_0^t dt_1 \dots \int_0^t dt_n \int_0^\infty ds_1 \dots \int_0^\infty ds_m \delta_{n+m+1}(t, t_1, \dots, t_n, s_1, \dots, s_m) = \frac{1}{n+1} \quad (2.55)$$

for a positive real number $t > 0$ and nonnegative integers $n, m \geq 0$ (see Appendix A.1.2 for derivation).

References

1. C.W. Gardiner, *Handbook of Stochastic Methods for Physics, Chemistry and the Natural Sciences*, 4th edn. (Springer, Berlin, 2009)
2. N.G. van Kampen, *Stochastic Processes in Physics and Chemistry*, 3rd edn. (North-Holland, Amsterdam, 2007)
3. P. Hänggi, *Z. Phys. B* **36**, 271 (1980)
4. H.-P. Breuer, F. Petruccione, *The Theory of Open Quantum Systems* (Oxford University Press, Oxford, 2002)
5. H. Risken, *The Fokker-Planck Equation*, 2nd edn. (Springer, Berlin, 1989)
6. H. Haken, *Synergetics: Introduction and Advanced Topics*, 3rd edn. (Springer, Berlin, 2004)
7. D. Applebaum, *Lévy Processes and Stochastic Calculus*, 2nd edn. (Cambridge University Press, Cambridge, 2009)
8. H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 5th edn. (World Scientific, Singapore, 2009)
9. N.G. van Kampen, *Can. J. Phys.* **39**, 551 (1961)
10. P. Hänggi, *Z. Phys. B* **31**, 407 (1978)

Statistical Mechanics for Athermal Fluctuation

Non-Gaussian Noise in Physics

Kanazawa, K.

2017, XVI, 222 p. 53 illus., 46 illus. in color., Hardcover

ISBN: 978-981-10-6330-5