Chapter 3
Random Walks and Mesoscopic Reaction–Transport Equations

As discussed in Sect. 2.1, the standard reaction–diffusion equation for the particle density $\rho(\mathbf{x}, t)$ has the form

$$\frac{\partial \rho}{\partial t} = D\Delta\rho + F(\rho), \qquad \mathbf{x} \in \mathbb{R}^3. \tag{3.1}$$

This equation is an example of a *macroscopic* reaction–transport equation that can be obtained in the long-time large-scale limit of *mesoscopic* equations. Recall that the *mesoscopic* approach is based on the idea that one can introduce mean-field equations for the particle density involving a detailed description of the movement of particles on the *microscopic* level. At the same time, random fluctuations around the mean behavior can be neglected due to a large number of individual particles. For example, we can obtain (3.1) from the mesoscopic integro-differential equation

$$\frac{\partial \rho}{\partial t} = \lambda \int_{\mathbb{R}^3} \rho(\mathbf{x} - \mathbf{z}, t) w(\mathbf{z}) \mathrm{d}\mathbf{z} - \lambda\rho(\mathbf{x}, t) + F(\rho), \tag{3.2}$$

where λ is the intensity of particle jumps and $w(\mathbf{z})$ is the long-distance dispersal kernel. This equation arises in population theory, where the dispersal of individuals leads to population spread in space and invasion into new territories. The reaction–diffusion equation (3.1) can also be obtained from the mesoscopic balance equations

$$\rho(\mathbf{x}, t) = \rho(\mathbf{x}, 0)\Psi(t) + \int_0^t j(\mathbf{x}, t - \tau)\Psi(\tau)\mathrm{d}\tau, \tag{3.3a}$$

$$j(\mathbf{x}, t) = F(\rho) + \int_{\mathbb{R}^3} \rho(\mathbf{x} - \mathbf{z}, 0)\psi(\mathbf{z}, t)\mathrm{d}\mathbf{z} + \\ + \int_0^t \int_{\mathbb{R}^3} j(\mathbf{x} - \mathbf{z}, t - \tau)\psi(\mathbf{z}, \tau)\mathrm{d}\mathbf{z}\mathrm{d}\tau. \tag{3.3b}$$

These are the mean-field equations for the density of particles that follow a continuous-time random walk (CTRW). Each random step of a particle is characterized by a waiting time and a jump length, which are distributed according to the joint

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probability density function (PDF) $\psi(\mathbf{z}, \tau)$. Here $j(\mathbf{x}, t)$ is the density of particles that are either produced with rate $F(\rho)$ at point $\mathbf{x}$ at time t or arrive there exactly at time t from other points $\mathbf{x} - \mathbf{z}$. The function

$$\Psi(t) = \int_t^\infty \int_{\mathbb{R}^3} \psi(\mathbf{z}, \tau) \mathrm{d}\mathbf{z}\mathrm{d}\tau \tag{3.4}$$

is the survival probability. Another long-time large-scale limit of (3.3) can be a fractional reaction–transport equation, such as

$$\frac{\partial \rho}{\partial t} = -D_\alpha (-\Delta)^{\frac{\alpha}{2}} \rho + F(\rho), \qquad \mathbf{x} \in \mathbb{R}^3, \tag{3.5}$$

where the Laplacian Δ is replaced by a fractional operator $-(-\Delta)^{\frac{\alpha}{2}}$ and D_α is a generalized diffusion coefficient. This replacement leads to a faster spread of particles, i.e., superdiffusion, see Sect. 3.3, than the standard reaction–diffusion equation (3.1) describes. The *microscopic* reason for the fast spread is that the jump length PDF

$$w(\mathbf{z}) = \int_0^\infty \psi(\mathbf{z}, \tau) \mathrm{d}\tau \tag{3.6}$$

has a heavy tail, so that $w(\mathbf{z}) \sim |\mathbf{z}|^{-d-\alpha}$ with $0 < \alpha < 2$ as $|\mathbf{z}| \to \infty$, where d is the dimension of space, $\mathbb{R}^d$. The fractional Laplacian can be defined as

$$(-\Delta)^{\frac{\alpha}{2}} g(\mathbf{x}) = \mathcal{F}^{-1}\left[|\mathbf{k}|^\alpha \tilde{g}(\mathbf{k})\right], \tag{3.7}$$

where $\mathcal{F}^{-1}$ denotes the inverse Fourier transform and $\tilde{g}(\mathbf{k}) = \mathcal{F}\left[g(\mathbf{x})\right] = \int_{\mathbb{R}^3} g(\mathbf{x})$ $\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} \mathrm{d}\mathbf{x}$. Fractional differential equations have attracted considerable interest in past years. We believe that the approach based on random walk models, the long-time large-scale limit asymptotics of mesoscopic equations, and stable distributions often provides a deeper insight into mechanisms by which the fractional equations arise than a standard phenomenological approach.

The main objective of this chapter is to establish the relation between the *macroscopic* equations like (3.1) and (3.5), the *mesoscopic* equations (3.2) and (3.3), etc., and the underlying *microscopic* movement of particles. We will show how to derive mesoscopic reaction–transport equations like (3.2) and (3.3) from microscopic random walk models. In particular, we will discuss the scaling procedures that lead to macroscopic reaction–transport equations. As an example, let us mention that the macroscopic reaction–diffusion equation (3.1) occurs as a result of the convergence of the random microscopic movement of particles to Brownian motion, while the macroscopic fractional equation (3.5) is closely related to the convergence of random walks with heavy-tailed jump PDFs to α-stable random processes or Lévy flights.

In the following section we restrict ourselves to one-dimensional models for expository purposes. The material is presented by means of examples of random walk models and corresponding mesoscopic equations and is sometimes supported by general theory.

3.1 Discrete-Time Random Walk

We begin with a simple example of a particle performing a discrete-time random walk (DTRW) in one dimension. Assume that it is initially at point 0. The random walk can be defined by the stochastic difference equation for the particle position X_n at time n:

$$X_{n+1} = X_n + Z_{n+1}, \tag{3.8}$$

where the jumps Z_n are mutually independent, continuous random variables with the common PDF

$$w(z) = \frac{\partial}{\partial z}\mathbb{P}(Z_n \leq z). \tag{3.9}$$

Equation (3.8) provides *a microscopic* description of the particle transport. After n jumps, the position of the particle is

$$X_n = \sum_{i=1}^{n} Z_i. \tag{3.10}$$

Let us define the PDF for the particle position X_n at time n:

$$p(x, n) = \frac{\partial}{\partial x}\mathbb{P}(X_n \leq x). \tag{3.11}$$

It follows from (3.8) and (3.9) that the PDF $p(x, n)$ obeys the Kolmogorov forward equation

$$p(x, n+1) = \int_{\mathbb{R}} p(x - z, n)w(z)\mathrm{d}z, \tag{3.12}$$

with $n = 0, 1, \ldots$. If Z_i has zero mean and finite variance, $\sigma^2 = \int_{\mathbb{R}} z^2 w(z)\mathrm{d}z$, the central limit theorem ensures that the PDF for the rescaled particle position $X_n/\sqrt{n}$ tends to a Gaussian as $n \to \infty$. If the jumps Z_n have a symmetric heavy-tailed PDF with power-law index $\alpha < 2$, then the variance σ^2 is infinite. According to the generalized central limit theorem, the rescaled position $X_n/n^{1/\alpha} \xrightarrow{\mathrm{d}} Z$ as $n \to \infty$,

where Z is a symmetric α-stable random variable and $\xrightarrow{\mathrm{d}}$ means convergence in distribution [126, 377].

3.1.1 Mesoscopic Equation for the Particle Density

Let us introduce the average density of particles $\rho(x, n)$ at point x at time n. We assume that the number of particles per unit length around x is large enough that we can neglect the random fluctuations in the number density. In this case, the particle density $\rho(x, n)$ obeys the integral balance equation

$$\rho(x, n+1) = \int_{\mathbb{R}} \rho(x - z, n) w(z) \mathrm{d}z. \tag{3.13}$$

This equation states that the particle density at time $n+1$ is the sum of the densities at intermediate points $x - z$ at time n multiplied by the probability of transition from $x - z$ to x. This is a *mesoscopic* description. Although it only deals with the mean density of particles $\rho(x, n)$, it involves a detailed description of the movement of particles on the *microscopic* level. Equation (3.13) is the same as the Kolmogorov forward equation (3.12). The solution to (3.13) can be rewritten as a convolution

$$\rho(x, n) = (\rho_0 * w^{*n})(x), \tag{3.14}$$

where $\rho_0(x)$ is the initial density, the asterisk $*$ denotes convolution, and $w^{*n} = w * \cdots * w$ (n times).

If the PDF is $w(x) = \frac{1}{2}\delta(x-a) + \frac{1}{2}\delta(x+a)$, jumps Z_n can take only two values, a and $-a$, with equal probabilities. In this case we have a recurrence equation

$$\rho(x, n+1) = \frac{1}{2}\rho(x - a, n) + \frac{1}{2}\rho(x + a, n). \tag{3.15}$$

This equation can be recognized as a finite difference approximation of the diffusion equation

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2}. \tag{3.16}$$

This becomes clearer if we let the time step be of size τ instead of size 1. Then the recurrence equation (3.15) can be rewritten as

$$\frac{\rho(x, t+\tau) - \rho(x, t)}{\tau} = D \frac{\rho(x + a, t) - \rho(x, t) + \rho(x - a, t)}{a^2}, \tag{3.17}$$

where t denotes a time point of the form $n\tau$ and $D = a^2/2\tau$. We see that (3.17) is a discrete version of the standard diffusion equation (2.1). Though trivial, this

derivation clearly explains the connection between the microscopic equation for a single particle (3.8), the mesoscopic description for the particle density (3.13), and the macroscopic diffusion equation (3.16). Later we discuss how the discrete random walk (3.8) converges to Brownian motion after rescaling the time and space steps, see Sect. 3.6.

So far we have considered a homogeneous-in-space random walk for which the jump size Z_{n+1} in (3.8) is independent of the particle position X_n. The natural generalization of this situation is the case where the jumps are described by the conditional PDF

$$w(z|x) = \frac{\partial}{\partial z}\mathbb{P}(Z_n \leq z|X_{n-1} = x). \tag{3.18}$$

The mesoscopic density is governed by the Kolmogorov forward equation, the Master equation,

$$\rho(x, n+1) = \int_{\mathbb{R}} \rho(x - z, n)w(z|x - z)\mathrm{d}z. \tag{3.19}$$

The discrete model has the advantage that it can be easily generalized to include various nonlinearities such as the kinetic term $F(\rho)$ and the dependence of the jump kernel w on the density ρ. In this case we have a nonlinear recurrence equation

$$\rho(x, n+1) = \int_{\mathbb{R}} F\left[\rho(x - z, n)\right] w(z|x - z, \rho(x - z, n))\mathrm{d}z, \tag{3.20}$$

with $n = 0, 1, 2, \ldots$.

3.1.2 Random Walk with Two States and the System of Two Mesoscopic Equations

So far we have considered a single *mesoscopic* equation for the particle density and a corresponding random walk model, a Markov process with continuous states in discrete time. It is natural to extend this analysis to a system of mesoscopic equations for the densities of particles $\rho_i(x, n)$, $i = 1, 2, \ldots, m$. To describe the *microscopic* movement of particles we need a vector process (X_n, S_n), where X_n is the position of the particle at time n and S_n its state at time n. S_n is a sequence of random variables taking one of m possible values at time n. One can introduce the probability density $p_i(x, n) = \partial\mathbb{P}(X_n \leq x, S_n = i)/\partial x$ and an imbedded Markov chain with the $m \times m$ transition matrix $\mathsf{H} = (h_{ij})$, so that the matrix entry h_{ij} corresponds to the conditional probability of a transition from state i to state j.

To illustrate the idea, we derive *mesoscopic* equations for two densities $\rho_i(x, n)$, $i = 1, 2$, at point x at time n. One can think of a particle that moves along the x-axis and that can be in two different states with dispersal kernels $w_1(z)$ and

$w_2(z)$. We assume that the particles either jump or change their state. If the particle is in state 1 at time n, then the probability of being in state 2 at time $n+1$ is h_{12}, and the probability of being in state 1 at time $n+1$ is $h_{11} = 1 - h_{12}$. In the same way, we can define the transition probabilities for the particle if it is in state 2 at time n. We assume that these probabilities are h_{21} and $h_{22} = 1 - h_{21}$. The transition matrix H of the Markov chain with two states has the form

$$\mathsf{H} = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix}. \tag{3.21}$$

The balance equations for the two densities $\rho_i(x, n)$, $i = 1, 2$, can be written as follows:

$$\rho_1(x, n+1) = h_{11} \int_{\mathbb{R}} \rho_1(x - z, n) w_1(z) \mathrm{d}z + h_{21} \rho_2(x, n), \tag{3.22a}$$

$$\rho_2(x, n+1) = h_{22} \int_{\mathbb{R}} \rho_2(x - z, n) w_2(z) \mathrm{d}z + h_{12} \rho_1(x, n), \tag{3.22b}$$

with $n = 0, 1, 2, \ldots$. The first equation states that the density of particles $\rho_1(x, n+1)$ in state 1 at point x at time $n+1$ is the sum of (i) the density of particles in state 1 at intermediate points $x - z$ at time n multiplied by the probability of remaining in state 1 at the transition time $n+1$ and the probability of transition from $x - z$ to x and (ii) the density of particles in state 2 at time n multiplied by the probability of transition from state 2 to state 1 at time $n+1$. It is straightforward to include kinetic terms $F_1(\rho_1)$ and $F_2(\rho_2)$ and the dependence of the transition probabilities h_{ij} on densities ρ_1 and ρ_2, similar to (3.20).

3.2 Continuous-Time Random Walk

We now turn to a particle that performs a random walk in continuous time. In order to keep this section as clear as possible, we will only consider one-dimensional random walk models. As before, we assume that the jumps $Z_1, Z_2, \ldots$ are independent identically distributed (IID) random variables. However, the jumps occur at random times $T_1, T_2, \ldots$, so that the intervals between jumps $\Theta_n = T_n - T_{n-1}$ are also IID variables. In general, the time intervals Θ_n and jumps Z_n are dependent, and their statistical characteristics are completely determined by the joint PDF $\psi(z, t)$. The spatial jump length PDF is given by $w(z) = \int_0^\infty \psi(z, t) \mathrm{d}t$ and the waiting time PDF by $\phi(t) = \int_{-\infty}^{\infty} \psi(z, t) \mathrm{d}z$. If jumps and waiting times are independent of each other, the corresponding joint PDF $\psi(z, t)$ factorizes:

$$\psi(z, t) = w(z) \phi(t). \tag{3.23}$$

Let $X(t)$ denote the position of the particle at time t and $X(0) = 0$, then

$$X(t) = \sum_{i=1}^{N(t)} Z_i, \tag{3.24}$$

where $N(t)$ is the number of jumps up to time t. It can be defined in terms of the random time T_n as follows:

$$N(t) = \max\left\{n \geq 0 : T_n \leq t\right\}. \tag{3.25}$$

Such a process $N(t)$ is called a *renewal* or *counting process*. The particle position $X(t)$ is called a *continuous-time random walk*. Figure 3.1 illustrates the process $X(t)$. It should be noted that the CTRW $X(t)$ defined by (3.24) can also be obtained by replacing the discrete time n in (3.10) with the "random" time $N(t)$, i.e.,

$$X(t) = X_{N(t)}. \tag{3.26}$$

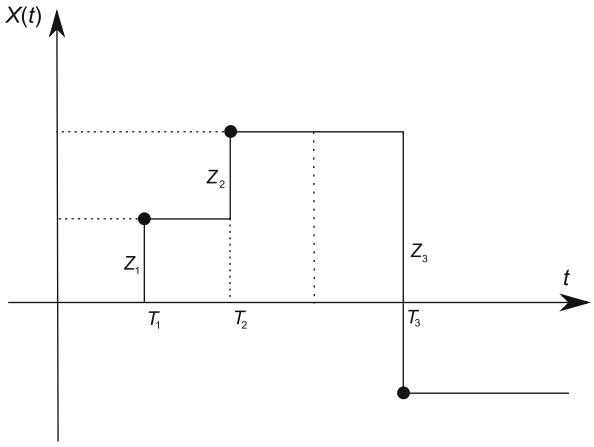

Fig. 3.1 Schematic picture of a CTRW

In the mathematical literature, $X(t)$ is called a *semi-Markov process* associated with the two-component Markov chain (X_n, T_n), a *Markov renewal process* [218]. As discussed in Sect. 2.3, the CTRW model is a standard approach for studying anomalous diffusion [298].

The *microscopic* stochastic equation for the particle position $X(t)$ can be written in the form

$$\frac{\mathrm{d}X}{\mathrm{d}t} = \sum_i Z_i \delta(t - T_i), \tag{3.27}$$

where the right-hand side represents the sum of the stochastic pulses at renewal times T_i with random amplitudes Z_i.

To find the PDF $p(x,t)$ for the particle position at time t we use the equation

$$p(x,t) = p_0(x)\Psi(t) + \int_0^t j(x,t-\tau)\Psi(\tau)\mathrm{d}\tau, \tag{3.28}$$

where $p_0(x)$ is the initial PDF, $j(x,t)$ is the probability density of reaching the point x exactly at time t, and

$$\Psi(t) = \int_t^\infty \int_{\mathbb{R}} \psi(z,\tau)\mathrm{d}z\mathrm{d}\tau \tag{3.29}$$

is the probability that the particle does not jump in the time interval $(0,t]$, i.e., the survival probability. Equation (3.28) expresses the law of total probability. The first term on the RHS of (3.28) represents the probability of being at the point x times the probability of no jumps up to time t. The second term takes into account the probability of arriving at the point x at time $t-\tau$ and the probability of no jumps during the remaining time τ. The density $j(x,t)$ obeys the balance equation

$$j(x,t) = \int_{\mathbb{R}} p_0(x-z)\psi(z,t)\mathrm{d}z + \int_0^t \int_{\mathbb{R}} j(x-z,t-\tau)\psi(z,\tau)\mathrm{d}z\mathrm{d}\tau. \tag{3.30}$$

Applying the Fourier–Laplace (F-L) transform to (3.28) and (3.30), we obtain the Fourier–Laplace transform of the PDF $p(x,t)$, the Montroll–Weiss equation,

$$\hat{\tilde{p}}(k,s) = \frac{\tilde{p}_0(k)\left[1-\hat{\phi}(s)\right]}{s\left[1-\hat{\tilde{\psi}}(k,s)\right]}. \tag{3.31}$$

Here $\hat{\phi}(s)$ is the Laplace transform of the waiting time PDF $\phi(t)$, $\tilde{p}_0(k)$ is the Fourier transform of the initial PDF $p_0(x)$, and $\hat{\tilde{\psi}}(k,s)$ is the F-L transform of the joint PDF $\psi(x,t)$. In particular, (3.31) can be rearranged for the uncoupled case (3.23) as

$$s\hat{\tilde{p}}(k,s) - \tilde{p}_0(k) = \frac{s\hat{\phi}(s)}{1-\hat{\phi}(s)}(\tilde{w}(k)-1)\hat{\tilde{p}}(k,s), \tag{3.32}$$

where the left-hand side is the Fourier–Laplace transform of the derivative $\partial p/\partial t$ and $\tilde{w}(k)$ is the Fourier transform of dispersal kernel $w(z)$. If we apply the F-L transform inversion, we obtain the integro-differential equation, the Master equation,

$$\frac{\partial p}{\partial t} = \int_0^t K(t-\tau)\left[\int_{\mathbb{R}} p(x-z,\tau)w(z)\mathrm{d}z - p(x,\tau)\right]\mathrm{d}\tau. \tag{3.33}$$

The memory kernel $K(t)$ is defined in terms of its Laplace transform, see (2.66),

$$\hat{K}(s) = \frac{\hat{\phi}(s)}{\hat{\Psi}(s)} = \frac{s\hat{\phi}(s)}{1-\hat{\phi}(s)}. \tag{3.34}$$

It should be emphasized that it is impossible to find an explicit expression for the memory kernel $K(t)$ for arbitrary choices of the waiting time PDF $\phi(t)$.

As we mentioned in Sect. 2.3, CTRWs can be characterized by the mean waiting time, $\overline{T} = \int_0^\infty t\phi(t)\mathrm{d}t$, and the second moment of the jump length PDF, $\sigma^2 = \int_{\mathbb{R}} z^2 w(z)\mathrm{d}z$. We assume that $w(z)$ is even, i.e., the first moment of $w(z)$ vanishes. If $\overline{T}$ and σ^2 are finite, the central limit theorem implies that the rescaled particle position $\sqrt{\varepsilon}X(t/\varepsilon)$ has a Gaussian PDF as $\varepsilon \to 0$,

$$\lim_{\varepsilon\to 0}\frac{\partial}{\partial x}\mathbb{P}\left(\sqrt{\varepsilon}X\left(\frac{t}{\varepsilon}\right)\le x\right) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right), \tag{3.35}$$

with $D = \sigma^2/2\overline{T}$. In another words, $\sqrt{\varepsilon}X(t/\varepsilon)$ converges in distribution to the Brownian motion $B(t)$ as $\varepsilon \to 0$.

The CTRW model is a standard tool for modeling subdiffusion, for which the variance of the particle position increases with time as t^γ with $0 < \gamma < 1$, see Sect. 2.3. This regime occurs if the waiting time PDF behaves like $\phi(t) \sim (\tau_0/t)^{1+\gamma}$ as $t \to \infty$. Then the mean waiting time $\overline{T}$ is infinite. The Laplace transform $\hat{\phi}(s)$ is approximated by

$$\hat{\phi}(s) \simeq 1 - (\tau_0 s)^\gamma \tag{3.36}$$

for small s and $0 < \gamma < 1$. Then $\hat{K}(s) \simeq s(\tau_0 s)^{-\gamma}$. Equation (3.32) can be written as $s^\gamma \hat{\tilde{p}}(k,s) - s^{\gamma-1}\tilde{p}_0(k) = \tau_0^{-\gamma}(\tilde{w}(k)-1)\hat{\tilde{p}}(k,s)$. We apply the F-L transform inversion and obtain the fractional Kolmogorov–Feller equation

$$\tau_0^\gamma \frac{\partial^\gamma p}{\partial t^\gamma} = \int_{\mathbb{R}} p(x-z,t)w(z)\mathrm{d}z - p(x,t), \tag{3.37}$$

where

$$\frac{\partial^\gamma p}{\partial t^\gamma} = \frac{1}{\Gamma(1-\gamma)}\frac{\partial}{\partial t}\int_0^t \frac{p(x,\tau)\mathrm{d}\tau}{(t-\tau)^\gamma} - \frac{t^{-\gamma}p_0(x)}{\Gamma(1-\gamma)} \tag{3.38}$$

is the Caputo fractional derivative, which reduces to the standard derivative for $\gamma = 1$.

3.2.1 Mesoscopic Equation for the Particle Density

Consider particles that undergo a continuous-time random walk and do not interact with each other. Then the balance equations for the mean density of particles $\rho(x,t)$ and the density of particles $j(x,t)$ arriving at the point x exactly at time t can be written as

$$\rho(x,t) = \rho_0(x)\Psi(t) + \int_0^t j(x,\tau)\Psi(t-\tau)\mathrm{d}\tau, \tag{3.39}$$

and

$$j(x,t) = \int_{\mathbb{R}} \rho_0(x-z)\psi(z,t)\mathrm{d}z + \int_0^t \int_{\mathbb{R}} j(x-z,\tau)\psi(z,t-\tau)\mathrm{d}z\mathrm{d}\tau, \tag{3.40}$$

where $\rho_0(x)$ is the initial particle density. These two equations have the same form as (3.28) and (3.30). The two balance equations (3.39) and (3.40) can be rewritten as a single equation:

$$\rho(x,t) = \rho_0(x)\Psi(t) + \int_0^t \int_{\mathbb{R}} \rho(x-z,\tau)\psi(z,t-\tau)\mathrm{d}z\mathrm{d}\tau. \tag{3.41}$$

Note that the initial distribution $\rho_0(x)$ is set up in such a way that the random walk for all particles starts from $t = 0$. Other choices of the time origin lead to aging effects [29]. In the following, we consider the uncoupled case (3.23) for simplicity. Using the Laplace–Fourier transform, we obtain from (3.39) and (3.40) the expression for $j(x,t)$ in terms of $\rho(x,t)$:

$$j(x,t) = \int_0^t \int_{\mathbb{R}} K(t-\tau)w(z)\rho(x-z,\tau)\mathrm{d}z\mathrm{d}\tau, \tag{3.42}$$

where the memory kernel $K(t)$ is given by (3.34). In the uncoupled case, (3.41) can be converted into the integro-differential transport equation, the generalized Master equation,

$$\frac{\partial \rho}{\partial t} = \int_0^t K(t-\tau)\left[\int_{\mathbb{R}} \rho(x-z,\tau)w(z)\mathrm{d}z - \rho(x,\tau)\right]\mathrm{d}\tau. \tag{3.43}$$

The intuitive meaning of the Master equation can be understood in terms of the density of particles $j(x,t)$ given by (3.42). If we differentiate $\rho(x,t)$ from (3.39) with respect to time, we obtain

$$\frac{\partial \rho}{\partial t} = -\rho_0(x)\phi(t) + j(x,t) - \int_0^t j(x,\tau)\phi(t-\tau)\mathrm{d}\tau, \tag{3.44}$$

since $\Psi'(t) = -\phi(t)$. The last equation can be written in the following form:

$$\frac{\partial \rho}{\partial t} = j(x,t) - i(x,t), \tag{3.45}$$

where $i(x,t)$ is the rate of departure of particles from the point x,

$$i(x,t) = \int_0^t K(t-\tau)\rho(x,\tau)\mathrm{d}\tau. \tag{3.46}$$

The generalized Master equation (3.43) can be rewritten as a simple rate equation:

$$\frac{\partial \rho}{\partial t} = \int_{\mathbb{R}} i(x-z,t)w(z)\mathrm{d}z - i(x,t). \tag{3.47}$$

It is tempting to generalize this equation by including a nonlinear reaction term $F(\rho)$ on its RHS:

$$\frac{\partial \rho}{\partial t} = \int_{\mathbb{R}} i(x-z,t)w(z)\mathrm{d}z - i(x,t) + F(\rho). \tag{3.48}$$

It turns out that the inclusion of the kinetic term $F(\rho)$ is not a trivial procedure for non-Markovian processes. In particular, the transport term might depend on the reaction kinetics. We discuss this problem later in detail, see Sect. 3.4.

As we mentioned, the particle position $X(t)$ can be expressed in terms of a discrete random walk X_n, see (3.10), and a counting process $N(t)$ as (3.26). Therefore, the solution of the Master equation (3.43) can be written as the average value

$$\rho(x,t) = \sum_{n=0}^{\infty} \rho(x,n)\mathbb{P}(N(t)=n), \tag{3.49}$$

where the density $\rho(x,n)$ is defined by the convolution equation (3.13). Here we have assumed that the jumps and waiting times are independent. Using the formula (3.14), we can express the particle density $\rho(x,t)$ in terms of the initial density $\rho_0(x)$ and the expectation operator $\mathbb{E}$ as

$$\rho(x,t) = \mathbb{E}\left(\rho_0 * w^{*N(t)}\right)(x) = \sum_{n=0}^{\infty} (\rho_0 * w^{*n})(x)\mathbb{P}(N(t)=n). \tag{3.50}$$

Applying the Fourier–Laplace transform, we obtain

$$\hat{\tilde{\rho}}(k,s) = \tilde{\rho}_0(k)\sum_{n=0}^{\infty} \tilde{w}^n(k)\hat{P}(n,s), \tag{3.51}$$

where $\hat{P}(n,s)$ is the Laplace transform of $P(n,t) = \mathbb{P}(N(t) = n)$. It is known from renewal theory [81] that

$$\hat{P}(n,s) = \frac{\hat{\phi}^n(s)\left[1 - \hat{\phi}(s)\right]}{s}. \tag{3.52}$$

Substitution of (3.52) into (3.51) yields

$$\hat{\tilde{\rho}}(k,s) = \frac{\tilde{\rho}_0(k)\left[1 - \hat{\phi}(s)\right]}{s} \sum_{n=0}^{\infty} \tilde{w}^n(k)\hat{\phi}^n(s) = \frac{\rho_0(k)\left[1 - \hat{\phi}(s)\right]}{s\left[1 - \tilde{w}(k)\hat{\phi}(s)\right]}, \tag{3.53}$$

which is exactly the formula (3.31) for the case $\hat{\tilde{\psi}}(k,s) = \tilde{w}(k)\hat{\phi}(s)$.

3.2.2 Random Walk with Discrete States in Continuous-Time

So far we have considered the homogeneous case for which the waiting time density is independent of the position of the particles or their state. Let us formulate the general equations describing a random walk with discrete states in continuous time for which the waiting time PDF depends on the current state. (CTRWs with space-dependent waiting time PDFs have been studied in [75].) We introduce the mean density of particles $\rho_m(t)$ in state m and the density of particles $j_m(t)$ arriving in state m exactly at time t. The balance equations can be written as

$$\rho_m(t) = \rho_{m0}\Psi_m(t) + \int_0^t j_m(\tau)\Psi_m(t-\tau)\mathrm{d}\tau \tag{3.54}$$

and

$$j_m(t) = \sum_{i\neq m} \rho_{i0}\phi_i(t)h_{im} + \sum_{i\neq m}\int_0^t j_i(\tau)\phi_i(t-\tau)h_{im}\mathrm{d}\tau. \tag{3.55}$$

Here $\Psi_m(t) = \int_t^\infty \phi_m(\tau)d\tau$ is the survival probability in the state m, h_{im} is the transition probability from state i to m, and ρ_{i0} is the initial density of particles in state i. Using the Laplace transform, we obtain from (3.54) and (3.55)

$$j_m(t) = \sum_{i\neq m}\int_0^t K_i(t-\tau)\rho_i(\tau)h_{im}\mathrm{d}\tau, \tag{3.56}$$

where the memory kernel $K_i(t)$ is defined in terms of its Laplace transform

$$\hat{K}_i(s) = \frac{\hat{\phi}_i(s)}{\hat{\Psi}_i(s)} = \frac{s\hat{\phi}_i(s)}{1 - \hat{\phi}_i(s)}. \tag{3.57}$$

The two balance equations can be rewritten as a single equation:

$$\rho_m(t) = \rho_{m0}\Psi_m(t) + \sum_{i\neq m}\int_0^t M_{im}(t-\tau)\rho_i(\tau)h_{im}\mathrm{d}\tau, \tag{3.58}$$

where the memory kernel $M_{im}(t)$ is defined as

$$\hat{M}_{im}(s) = \frac{\hat{\phi}_i(s)\hat{\Psi}_m(s)}{\hat{\Psi}_i(s)}. \tag{3.59}$$

It should be noted that (3.58) cannot be written in the standard form (3.41), which makes it difficult to give its probabilistic interpretation.

The generalized Master equation is

$$\frac{\partial\rho_m(t)}{\partial t} = \sum_{i\neq m}\int_0^t K_i(t-\tau)\rho_i(\tau)h_{im}\mathrm{d}\tau - \int_0^t K_m(t-\tau)\rho_m(\tau)\mathrm{d}\tau. \tag{3.60}$$

This equation can be useful for studying multi-component systems where the chemical reactions do not obey classical kinetics.

3.2.3 Semi-Markov Processes

As mentioned on page 61, CTRWs are known as semi-Markov processes in the mathematical literature. In this section we provide a brief account of semi-Markov processes. They were introduced by P. Lévy and W. L. Smith [253, 415]. Recall that for a continuous-time Markov chain, the transitions between states at random times T_n are determined by the discrete chain X_n with the transition matrix $\mathsf{H} = (h_{ij})$. The waiting time $\Theta_n = T_n - T_{n-1}$ for a given state i is exponentially distributed with the transition rate λ_i, which depends only on the current state i. The natural generalization is to allow arbitrary distributions for the waiting times. This leads to a semi-Markov process. The reason for such a name is that the underlying process is a two-component Markov chain: (X_n, T_n). Here the random sequence X_n represents the state at the nth transition, and T_n is the time of the nth transition. Obviously, $T_n = \sum_{k=1}^n \Theta_k$.

The main statistical characteristic of the two-component Markov chain (X_n, T_n) is the transition kernel

$$Q_{ij}(t) = \mathbb{P}\left\{X_{n+1} = j, \Theta_{n+1} \leq t | X_n = i\right\} \tag{3.61}$$

for any $n \geq 0$. Here we consider only time-homogeneous chains for which the kernel $Q_{ij}(t)$ is independent of n. We use the counting process $N(t)$ (3.25) that gives the number of transitions in the time interval $(0, t]$.

Semi-Markov processes can be defined as

$$X(t) = X_{N(t)} \tag{3.62}$$

or

$$X(t) = X_n \quad \text{if} \quad T_n \leq t < T_{n+1}. \tag{3.63}$$

If the process starts in the state i, then the subsequent state j is determined by the transition kernel Q so that the process remains in state i some random time before making a transition to j. One can introduce the conditional waiting time distribution $\Phi_{ij}(t)$ as

$$\Phi_{ij}(t) = \mathbb{P}\left\{T_{n+1} - T_n \leq t | X_n = i,\ X_{n+1} = j\right\}. \tag{3.64}$$

It gives us the distribution of the random time spent in state i before jumping to state j. The transition kernel $Q_{ij}(t)$ can be written as

$$Q_{ij}(t) = h_{ij}\Phi_{ij}(t), \tag{3.65}$$

where h_{ij} is the transition probability matrix of the underlying discrete Markov chain X_n. Note that $Q_{ij}(t) \to h_{ij}$ as $t \to \infty$ since $\Phi_{ij}(\infty) = 1$. In general, the waiting time distribution depends on the current state i and the next state j.

The standard continuous-time Markov chain is a special case of a semi-Markov process with the transition kernel

$$Q_{ij}(t) = h_{ij}(1 - \exp(-\lambda_i t)). \tag{3.66}$$

The transition probability

$$p_{ij}(t) = \mathbb{P}\{X(t) = j | X(0) = i\} \tag{3.67}$$

satisfies the integral backward equation

$$p_{ij}(t) = \delta_{ij} S_i(t) + \sum_k \int_0^t q_{ik}(t - \tau) p_{kj}(\tau) \mathrm{d}\tau, \tag{3.68}$$

where

$$q_{ij}(t) = \frac{\partial Q_{ij}(t)}{\partial t} \tag{3.69}$$

is the transition density kernel and

$$S_i(t) = 1 - \sum_k Q_{ik}(t) \tag{3.70}$$

is the survival probability for state i. The first term $\delta_{ij} S_i(t)$ in (3.68) represents the probability that the process $X(t)$ does not leave the state i up to time t, given that it was in this state initially. In the Markovian case, $q_{ij}(t) = \lambda_i \exp(-\lambda_i t) h_{ij}$, this equation is equivalent to a system of backward differential equations for Markov processes. Janssen and Manca have summarized the theory of semi-Markov processes and discussed its applications in [218].

3.3 Markov CTRW Models

3.3.1 Compound Poisson Process

If the counting process $N(t)$ is a Poisson process with the transition rate λ, then the particle position

$$X(t) = \sum_{i=1}^{N(t)} Z_i \tag{3.71}$$

is a compound Poisson process [126]. The probability that n jumps occur in the time interval $[0, t]$ is given by

$$\mathbb{P}(N(t) = n) = \frac{(\lambda t)^n}{n!} \mathrm{e}^{-\lambda t}. \tag{3.72}$$

Note that the Poisson process plays a very important role in random walk theory. It can be defined in two ways: (1) as a continuous-time Markov chain with constant intensity, i.e., as a pure birth process with constant birth rate λ; (2) as a renewal process. In the latter case, it can be represented as (3.25) with $T_n = \sum_{i=0}^{n} \Theta_i$. Here Θ_i are interarrival (waiting) times, which are independent random variables with PDF

$$\phi(t) = \lambda \mathrm{e}^{-\lambda t}. \tag{3.73}$$

Since the waiting time PDF $\phi(t)$ is exponential, the random walk $X(t)$ is a Markov process. The jump PDF $w(z)$ is defined in (3.9).

The *mesoscopic* particle density $\rho(x, t)$ obeys the integro-differential equation

$$\frac{\partial \rho}{\partial t} = \lambda \int_{\mathbb{R}} \rho(x - z, t) w(z) \mathrm{d}z - \lambda \rho(x, t). \tag{3.74}$$

The integro-differential equation (3.74) can be derived in several ways. The following is probably the most instructive in the context of transport theory. Since a compound Poisson process is Markovian, the derivation of (3.74) is based on the idea that the particle density at time $t + h$ can be expressed in terms of the density

at time t. In other words, the balance of particles during time $(t, t+h]$ is independent of what happened during the previous time interval $(0, t]$. We assume that the probability of a jump during a small time interval of length h is $\lambda h + o(h)$ and the probability of no jumps is $1 - \lambda h + o(h)$. Thus the balance of particles at the point x can be written as

$$\rho(x, t+h) = (1 - \lambda h)\rho(x, t) + \lambda h \int_{\mathbb{R}} \rho(x - z, t) w(z) \mathrm{d}z. \tag{3.75}$$

Subtracting $\rho(x, t)$ from both sides of this equation, dividing by h, and letting $h \to 0$, we obtain (3.74). Obviously, (3.74) corresponds to a particular case of (3.43), namely where the time integral disappears, i.e., the Markov case.

Since the process is Markovian, it is easy to include chemical reactions in the above model by adding the kinetic term $F(\rho)h$ to the RHS of (3.75):

$$\frac{\partial \rho}{\partial t} = \lambda \int_{\mathbb{R}} \rho(x - z, t) w(z) \mathrm{d}z - \lambda \rho(x, t) + F(\rho). \tag{3.76}$$

We can rewrite this equation with the initial condition $\rho(x, 0) = \rho_0(x)$ in integral form. Let us look at (3.76) as a first-order inhomogeneous ODE of the form $\mathrm{d}\rho/\mathrm{d}t = -\lambda\rho(t) + g(t)$, where the function $g(t)$ combines the integral term and the kinetic term $F(\rho)$. This equation has a solution $\rho(t) = \rho(0)\mathrm{e}^{-\lambda t} + \int_0^t g(t - \tau)\mathrm{e}^{-\lambda\tau}\mathrm{d}\tau$, which implies that

$$\begin{aligned} \rho(x, t) = \rho_0(x)\mathrm{e}^{-\lambda t} &+ \int_0^t \int_{\mathbb{R}} \rho(x - z, t - \tau) w(z) \lambda \mathrm{e}^{-\lambda\tau} \mathrm{d}z \mathrm{d}\tau \\ &+ \int_0^t F(\rho(x, t - \tau))\mathrm{e}^{-\lambda\tau}\mathrm{d}\tau. \end{aligned} \tag{3.77}$$

The first term on the right-hand side represents those particles that stay at point x up to time t. The exponential factor $\mathrm{e}^{-\lambda t} = 1 - \int_0^t \phi(\tau)\mathrm{d}\tau$ is the probability that the particle makes no jump until time t. This is the survival probability $\Psi(t)$ for $\phi(t) = \lambda\mathrm{e}^{-\lambda t}$. The second term includes the contribution from the particles jumping to point x from different positions $x - z$ at time $t - \tau$ and surviving up to time t. The last term describes the contribution from the chemical reaction with the rate $F(\rho)$.

The natural generalization of a compound Poisson process is the *Markov jump process* $X(t)$ with the following statistical properties. If the position of a particle at time t is $X(t)$, then the probability of a jump during a small time interval $(t, t+h]$ is $\lambda(X(t))h + o(h)$, so that $X(t+h) = X(t) + Z(t) + o(h)$. The probability of no jump during $(t, t+h]$ is $1 - \lambda(X(t))h + o(h)$. The conditional density for a stationary jump process $Z(t)$ is

$$w(z|x) = \frac{\partial}{\partial z}\mathbb{P}\left\{Z(t) \le z | X(t) = x\right\}. \tag{3.78}$$

The balance of particles at the point x is

$$\rho(x,t+h) = \int_{\mathbb{R}} \rho(x-z,t)\lambda(x-z)hw(z|x-z)\mathrm{d}z + (1-\lambda(x)h)\rho(x,t) + o(h). \tag{3.79}$$

Subtracting $\rho(x,t)$ from both sides, dividing by h, and letting $h \to 0$, we obtain the mesoscopic equation, the Master equation,

$$\frac{\partial\rho(x,t)}{\partial t} = \int_{\mathbb{R}} \rho(x-z,t)\lambda(x-z)w(z|x-z)\mathrm{d}z - \lambda(x)\rho(x,t). \tag{3.80}$$

This equation can easily be generalized to include various nonlinear effects. In particular, the jump PDF $w(z|x)$ and the jump rate $\lambda(x)$ can depend on the local density $\rho(x,t)$, due to an overcrowding effect for example. Then

$$\frac{\partial\rho(x,t)}{\partial t} = \int_{\mathbb{R}} \rho(x-z,t)\lambda(x-z,\rho(x-z,t))w(z|x-z,\rho(x-z,t))\mathrm{d}z - \lambda(x,\rho(x,t))\rho(x,t) + F(\rho). \tag{3.81}$$

3.3.2 System of Two Mesoscopic Equations

We consider the transport of particles A and B with linear reversible reaction A $\rightleftharpoons$ B. One can introduce a two-component system of equations for the densities $\rho_1(x,t)$ and $\rho_2(x,t)$. We assume that the probability of a transition from A to B during a small time interval of length h is $\alpha_1 h + o(h)$, and the backward transformation B $\longrightarrow$ A has the probability $\alpha_2 h + o(h)$. We assume that the reaction is independent of the transport of particles. The probability of a jump during a small time interval h is $\lambda_1 h + o(h)$ for particles A and $\lambda_2 h + o(h)$ for particles B. The balance of particles A and B at the point x can be written as

$$\rho_1(x,t+h) = (1-\lambda_1 h - \alpha_1 h)\rho_1(x,t) + \lambda_1 h \int_{\mathbb{R}} \rho_1(x-z,t)w_1(z)\mathrm{d}z + \alpha_2 h\rho_2(x,t) + o(h), \tag{3.82a}$$

$$\rho_2(x,t+h) = (1-\lambda_2 h - \alpha_2 h)\rho_2(x,t) + \lambda_2 h \int_{\mathbb{R}} \rho_2(x-z,t)w_2(z)\mathrm{d}z + \alpha_1 h\rho_1(x,t) + o(h). \tag{3.82b}$$

These equations are the conservation laws for A and B particles. The first term on the right-hand side of (3.82a) represents the particles A that stay at location x and do not move during the time interval $(t, t+h]$ and do not become particles B. The second term corresponds to the number of particles of type A that arrive at x during $(t, t+h]$ from other points $x-z$, where the jump length z is distributed according to

the dispersal kernel or jump length PDF $w_1(z)$. The last term represents the number of particles B that turn into particles of type A.

In the limit $h \to 0$, we obtain the mesoscopic system of reaction–transport equations

$$\frac{\partial \rho_1}{\partial t} = \lambda_1 \int_{\mathbb{R}} \rho_1(x - z, t) w_1(z) \mathrm{d}z - \lambda_1 \rho_1 - \alpha_1 \rho_1 + \alpha_2 \rho_2, \tag{3.83a}$$

$$\frac{\partial \rho_2}{\partial t} = \lambda_2 \int_{\mathbb{R}} \rho_2(x - z, t) w_2(z) \mathrm{d}z - \lambda_2 \rho_2 + \alpha_1 \rho_1 - \alpha_2 \rho_2. \tag{3.83b}$$

The main advantage of this Markovian model is that it can be easily generalized to include various nonlinear terms. Later we consider non-Markovian models for which the inclusion of nonlinear effects is a highly nontrivial procedure, see Sect. 3.4.

3.3.3 Characteristic Function and Transport Equation for the Particle Density

Characteristic functions are very useful tools for studying random processes. It turns out that reaction–transport equations can also be effectively handled by using the characteristic function of the underlying random walks. In what follows, we will see how this function helps to define the transport operator, a pseudo-differential operator, for the mean density $\rho(x, t)$.

3.3.3.1 Compound Poisson process

For illustrative purposes we begin with the transport of particles that follow the path of the compound Poisson process (3.71), $X(t) = \sum_{i=1}^{N(t)} Z_i$. The corresponding mean-field equation for the density $\rho(x, t)$ is given by (3.74). Let us show that this equation is closely related to the characteristic function $\tilde{\rho}(k, t)$ of $X(t)$:

$$\tilde{\rho}(k, t) = \mathbb{E}\left(\mathrm{e}^{\mathrm{i}kX(t)}\right) = \sum_{n=0}^{\infty} \mathbb{E}\left(\mathrm{e}^{\mathrm{i}kX(t)} \big| N(t) = n\right) \mathbb{P}(N(t) = n). \tag{3.84}$$

Here $\mathbb{P}(N(t) = n) = \mathrm{e}^{-\lambda t} \frac{(\lambda t)^n}{n!}$, and the conditional expectation is given by

$$\mathbb{E}\left(\mathrm{e}^{\mathrm{i}kX(t)} \big| N(t) = n\right) = \mathbb{E}\left(\mathrm{e}^{\mathrm{i}k \sum_{i=1}^{n} Z_i} \big| N(t) = n\right) = \tilde{w}^n(k), \tag{3.85}$$

where $\tilde{w}(k)$ is the characteristic function of the random jump Z_i with the density $w(z)$,

$$\tilde{w}(k) = \mathbb{E}\left(\mathrm{e}^{\mathrm{i}kZ_i}\right) = \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}kz} w(z) \mathrm{d}z. \tag{3.86}$$

We obtain

$$\tilde{\rho}(k,t) = \sum_{n=0}^{\infty} \mathrm{e}^{-\lambda t} \frac{(\lambda t \tilde{w}(k))^n}{n!} = \mathrm{e}^{t\psi(k)}, \tag{3.87}$$

where

$$\psi(k) = \lambda(\tilde{w}(k) - 1) \tag{3.88}$$

is the characteristic exponent of the compound Poisson process $X(t)$. Note that $\psi(k) = -Dk^2$ corresponds to the Brownian motion $B(t)$ and $\psi(k) = \mathrm{i}kv - Dk^2$ is the characteristic exponent of the Brownian motion with drift vt.

The function $\psi(k)$ plays a very important role in defining a transport operator. It follows from (3.87) that the function $\tilde{\rho}(k,t)$ satisfies the equation

$$\frac{\partial \tilde{\rho}(k,t)}{\partial t} = \psi(k)\tilde{\rho}(k,t). \tag{3.89}$$

Applying the inverse Fourier transform to (3.89) with (3.88) and the standard convolution theorem, we obtain the Kolmogorov–Feller equation (3.74). Thus the particle density $\rho(x,t)$ can be interpreted as the inverse Fourier transform of the characteristic function $\tilde{\rho}(k,t) = \mathbb{E}(\mathrm{e}^{\mathrm{i}kX(t)})$. Since $\tilde{\rho}(k,0) = 1$, the initial particle density is $\rho(x,0) = \delta(x)$. The integral operator on the RHS of the Kolmogorov–Feller equation (3.74) can be considered as a pseudo-differential operator with symbol (3.88). Recall that a pseudo-differential operator L_x acting on the variable x is defined by its Fourier transform as $\mathcal{F}[L_x\rho(x,t)] = \psi(k)\tilde{\rho}(k,t)$, where $\psi(k)$ is referred to as the symbol of L_x (see, for example, [15]).

3.3.3.2 Symmetric α-Stable Lévy Process

Let us now consider another example of a Markov process for which the characteristic exponent is

$$\psi(k) = -D_\alpha |k|^\alpha, \quad 0 < \alpha < 2. \tag{3.90}$$

This exponent corresponds to a symmetric α-stable Lévy process $S_\alpha(t)$, a Lévy flight, which is self-similar with Hurst exponent $H = 1/\alpha$. It follows from (3.89) that the mesoscopic density of particles is the solution to the space-fractional diffusion equation [371]:

$$\frac{\partial \rho(x,t)}{\partial t} = D_\alpha \frac{\partial^\alpha \rho(x,t)}{\partial |x|^\alpha}, \tag{3.91}$$

where D_α is a generalized diffusion coefficient and $\partial^\alpha \rho(x,t)/\partial |x|^\alpha$ is the symmetric Riesz fractional derivative of order α defined by the Fourier representation

$$\mathcal{F}\left[\frac{\partial^{\alpha}\rho(x,t)}{\partial\,|x|^{\alpha}}\right] = -\,|k|^{\alpha}\,\tilde{\rho}(k,t). \tag{3.92}$$

The symmetric Riesz fractional derivative (3.92) is the pseudo-differential operator with symbol $-\,|k|^{\alpha}$. Such a derivative describes a redistribution of particles in the whole space according to the heavy-tailed distribution of the jumps

$$\mathbb{P}\{|Z_i| > z\} \sim \frac{A}{z^{\alpha}}, \tag{3.93}$$

for large z. The symmetric Riesz derivative can be represented in explicit form as [371, 372]

$$\frac{\partial^{\alpha}\rho(x,t)}{\partial\,|x|^{\alpha}} = \frac{\Gamma(1+\alpha)}{\pi}\sin\left(\frac{\alpha\pi}{2}\right)\int_0^{\infty}\frac{\rho(x-z,t)-2\rho(x,t)+\rho(x+z,t)}{z^{1+\alpha}}\mathrm{d}z. \tag{3.94}$$

The space-fractional equation (3.91) can be derived from the Kolmogorov–Feller equation (3.74) by using the assumption that the random jump Z_i has a Lévy-stable PDF $w_{\alpha}(z)$, symmetric with respect to zero, with power-law tails as $z \to \infty$. There is no general explicit form for $w_{\alpha}(z)$, but the characteristic function of $w_{\alpha}(z)$, the structure function, is

$$\tilde{w}_{\alpha}(k) = \mathrm{e}^{-\sigma^{\alpha}|k|^{\alpha}}. \tag{3.95}$$

The width of the density $w_{\alpha}(z)$ cannot be measured by the variance $\int_{\mathbb{R}} z^2 w_{\alpha}(z)dz$, which is infinite for $\alpha < 2$. The function $w_{\alpha}(z)$ looks similar to a normal density in the center, but the tails of $w_{\alpha}(z)$ are much flatter than those of a Gaussian distribution. The asymptotic expression for large $|z|$ involves power-law tails:

$$w_{\alpha}(z) \sim \frac{\sigma^{\alpha}\Gamma(1+\alpha)\sin(\alpha\pi/2)}{\pi}\,|z|^{-1-\alpha} \tag{3.96}$$

(see, for example, [126, 373]). We show using scaling arguments that the large-scale long-time limit for $\rho(x,t)$ is the symmetric α-stable density that decays like $t\,|x|^{-1-\alpha}$ as $x \to \infty$. It follows from (3.88) and (3.89) that $\tilde{\rho}(k,t)$ satisfies

$$\frac{\partial\tilde{\rho}(k,t)}{\partial t} = \lambda\left(\mathrm{e}^{-\sigma^{\alpha}|k|^{\alpha}} - 1\right)\tilde{\rho}(k,t). \tag{3.97}$$

Let us find a space–time scaling, $k \to \varepsilon^{H}k$ and $t \to t/\varepsilon$, for which the characteristic function

$$\tilde{\rho}^{*}(k,t) = \lim_{\varepsilon\to 0}\tilde{\rho}^{\varepsilon}(k,t) = \lim_{\varepsilon\to 0}\tilde{\rho}\left(\varepsilon^{H}k, \frac{t}{\varepsilon}\right) \tag{3.98}$$

is scale invariant. In what follows we omit the asterisk for $\tilde{\rho}^*(k,t)$. From (3.97) and (3.98) we find that

$$\tilde{\rho}(k,t) = \lim_{\varepsilon \to 0} \exp\left[\frac{\lambda t}{\varepsilon}\left(\mathrm{e}^{-\sigma^\alpha |k|^\alpha \varepsilon^{H\alpha}} - 1\right)\right] = \exp\left(-\lambda \sigma^\alpha |k|^\alpha t\right) \tag{3.99}$$

for the Hurst exponent $H = \alpha^{-1}$. In this case, $\rho(x,t) = \mathcal{F}^{-1}[\tilde{\rho}(k,t)]$ is the solution to the space-fractional equation (3.91) with $D_\alpha = \lambda \sigma^\alpha$. Let us find this solution by using the scaling rules for the Fourier transform: $g(x/a) \overset{\mathcal{F}}{\to} a\tilde{g}(ak)$. If we set $\lambda = 1$ and $a = t^{1/\alpha}$, then it follows from (3.99) and (3.95) that the Green's function $G(x,t)$ for the space-fractional equation (3.91) with $\rho(x,0) = \delta(x)$ can be written in terms of the symmetric Lévy-stable PDF $w_\alpha(z)$ as

$$G(x,t) = t^{-\frac{1}{\alpha}} w_\alpha\left(x t^{-\frac{1}{\alpha}}\right). \tag{3.100}$$

The Cauchy problem for (3.91) with $\rho(x,0) = \rho_0(x)$ has the solution

$$\rho(x,t) = \int_{\mathbb{R}} G(x-z,t)\rho_0(z)\mathrm{d}z. \tag{3.101}$$

Note that an asymmetric density of jump lengths leads to the Riesz–Feller space-fractional derivative of order α and skewness θ with the characteristic exponent

$$\psi(k) = -D_\alpha |k|^\alpha \mathrm{e}^{\mathrm{i}\,\mathrm{sgn}(k)\theta\pi/2}, \quad 0 < \alpha < 2, \quad |\theta| \le \min\{\alpha, 2-\alpha\}. \tag{3.102}$$

The Cauchy problem involving the Riesz–Feller derivative was analyzed in [166, 260]. In the next section we discuss the general Markov random processes with independent and stationary increments, the Lévy processes, for which the characteristic function is known explicitly.

3.3.4 Lévy Processes

In the previous two sections we gave a brief account of the compound Poisson process and the symmetric α-stable Lévy process. This section is an introduction to general one-dimensional Lévy processes. The compound Poisson process and symmetric α-stable process are simply examples of Markov processes of Lévy type. Readers who are interested in this topic in greater detail are referred to the books by Applebaum [15] and Sato [378].

Recall that a Lévy process $X(t)$ is a continuous-time stochastic process that has independent and stationary increments. It represents a natural generalization of a simple random walk defined as a sum of independent identically distributed random variables. The independence of increments ensures that Lévy processes are Markov processes. The main feature of a Lévy process is that it is infinitely divisible for

any time t. It can be written as a sum of increments $X(t) = \sum_{k=1}^{n} \Delta X^k(t)$ for any $n \in N$, where $\Delta X^k(t)$ are identically distributed random variables. It is usually assumed that $X(0) = 0$. The simplest examples of Lévy processes are the Brownian motion $B(t)$, the Poisson process $N(t)$, and the compound Poisson process $X(t)$. Any Lévy process $X(t)$ can be written as the sum of a drift term at, a Brownian motion $B(t)$, and a pure jump process $Z(t)$ with a finite or infinite number of jumps in the interval $[0, t]$.

Its statistical characteristics are completely determined by the characteristic exponent $\psi(k)$, defined as

$$\mathbb{E}\left\{\mathrm{e}^{\mathrm{i}kX(t)}\right\} = \mathrm{e}^{t\psi(k)}. \tag{3.103}$$

The exponent $\psi(k)$ has the Lévy–Khinchine representation

$$\psi(k) = \mathrm{i}ak - Dk^2 + \int_{z\neq 0} \left(\mathrm{e}^{\mathrm{i}kz} - 1 - \mathrm{i}kz\chi_{0<|z|<1}\right) \nu(\mathrm{d}z), \tag{3.104}$$

where a and D are constants, χ_A is the indicator function of the set A, and $\nu(\mathrm{d}z)$ is a Lévy measure. The positive measure $\nu(A)$ is defined as the expected number of jumps of $X(t)$ per unit time, whose sizes belong to the set A. It must satisfy the integrability condition $\int_{z\neq 0} \min(1, z^2)\nu(dz) < \infty$, which means that there is a finite number of jumps whose size is $|z| \geq 1$, $\int_{|z|\geq 1} \nu(dz) < \infty$, and $\int_{0<|z|<1} z^2\nu(dz) < \infty$ because of the convergence requirement for the integral in (3.104). For example, the Lévy measure for the compound Poisson process (3.71) is $\nu(\mathrm{d}z) = \lambda w(z)\mathrm{d}z$. Note that instead of $z\chi_{0<|z|<1}$ one can use any bounded continuous function $g(z)$ satisfying $g(z) \to z$ as $z \to 0$. For example, $g(z) = z/(1 + z^2)$ or $g(z) = \sin z$.

It follows from the previous section that the Fourier transform $\tilde{\rho}(k, t)$ of the particle density $\rho(x, t)$ satisfies the equation

$$\frac{\partial \tilde{\rho}(k, t)}{\partial t} = \psi(k)\tilde{\rho}(k, t). \tag{3.105}$$

If we apply the inverse Fourier transform to this equation, we obtain an equation for the density $\rho(x, t)$:

$$\frac{\partial \rho}{\partial t} + a\frac{\partial \rho}{\partial x} = D\frac{\partial^2 \rho}{\partial x^2} + \int_{z\neq 0} \left(\rho(x - z, t) - \rho(x, t) + z\frac{\partial \rho}{\partial x}\chi_{0<|z|<1}\right) \nu(\mathrm{d}z). \tag{3.106}$$

In particular, if the Lévy measure is $\nu(\mathrm{d}z) = \lambda\delta(z - z_0)\mathrm{d}z$ and the size of the jumps is $z_0 > 1$, then

$$\psi(k) = \mathrm{i}ak - Dk^2 + \lambda\left(\mathrm{e}^{\mathrm{i}kz_0} - 1\right). \tag{3.107}$$

The intuitive meaning of this formula is as follows. Let $X(t)$ be the position of a particle performing a random Lévy walk with (3.107), then $X(t) = at + B(t) + N_z(t)$. The particle starts at zero and then follows the Brownian motion $B(t)$ with the drift velocity a until the random time T_1 at which a jump of size z_0 takes place. Between random times T_1 and T_2 we have again the Brownian motion with a drift and then another jump of the same size z_0 at time T_2. The last term in (3.107) is related to a Poisson process $N_z(t)$ with the rate λ in the set of values $\{nz_0\}$ with $n = 1, 2, \ldots$. The particle position $X(t)$ is an example of a *cadlag* function. It is a *right-continuous with left limits* function for which there exist two limits, $X(t^+) = \lim_{s\to t^+} X(s)$ and $X(t^-) = \lim_{s\to t^-} X(s)$, so that $X(t) = X(t^+)$. The difference $\Delta X = X(t) - X(t^-)$ describes the jump of $X(t)$ at time t.

For example, the Lévy measure corresponding to anomalous transport is

$$\nu(\mathrm{d}z) = \frac{C\,\mathrm{d}z}{|z|^{1+\alpha}} \tag{3.108}$$

where $C = \text{const}$, $0 < \alpha < 2, \alpha \neq 1$ and $z \neq 0$. Let us assume that the drift a and the diffusion coefficient D are zero. Then it follows from (3.104) and (3.108) that the particle position $X(t)$ is the symmetric α-stable random process $S_\alpha(t)$, sometimes called a Lévy flight, with the anomalous diffusion coefficient $D_\alpha = 2C\alpha^{-1}\Gamma(1-\alpha)\cos(\pi\alpha/2)$, see Sect. 3.3.3.2. It has an infinite variance which is associated with very large jumps. The mesoscopic transport equation for the particle density $\rho(x, t)$ is the space-fractional diffusion equation (3.91).

3.3.4.1 Finite and Infinite Number of Jumps

We can distinguish two cases: (1) the average number of jumps is finite, i.e., $\int_{z\neq 0} \nu(\mathrm{d}z) < \infty$; (2) infinite number of jumps, i.e., $\int_{z\neq 0} \nu(\mathrm{d}z) = \infty$.

The *compound Poisson process* $X(t)$, defined by (3.71), is an example of a pure jump process which has only a finite number of jumps on the finite time interval $[0, t]$. The Lévy measure $\nu(\mathrm{d}z) = \lambda w(z)\mathrm{d}z$ is finite on $\mathbb{R}$, that is, $\int_{z\neq 0} \nu(\mathrm{d}z) = \lambda < \infty$. Note that ν is not a probability measure, because $\int_{\mathbb{R}} \nu(\mathrm{d}z) = \lambda$. The characteristic function for the compound Poisson process is

$$\tilde{\rho}(k, t) = \mathrm{e}^{t\lambda(\tilde{w}(k)-1)} = \mathrm{e}^{t\psi(k)}, \tag{3.109}$$

where $\psi(k)$ is the characteristic exponent (see also (3.88))

$$\psi(k) = \lambda \int_{\mathbb{R}} \left(\mathrm{e}^{\mathrm{i}kz} - 1\right) w(z)\mathrm{d}z. \tag{3.110}$$

The mesoscopic density of particles obeys the integro-differential equation (3.74).

The *Gamma process* is an example of a Lévy process with infinite number of jumps. The Gamma process $X_\Gamma(t)$ is a pure jump Lévy process with the intensity measure

$$\nu(\mathrm{d}z) = \frac{\gamma_0}{z}\mathrm{e}^{-\beta z}\mathrm{d}z, \quad z > 0. \tag{3.111}$$

The jumps in $X_\Gamma(t)$ with a size in the interval $[z, z + \mathrm{d}z]$ occur $\nu(\mathrm{d}z)$. The parameter γ_0 determines the rate of jumps per unit time and β is the measure of jump size. Since the jumps are positive, we analyze the Gamma process by using the Laplace transform

$$\mathbb{E}\left\{\mathrm{e}^{-sX_\Gamma(t)}\right\} = \mathrm{e}^{t\int_0^\infty(\mathrm{e}^{-sz}-1)\nu(\mathrm{d}z)}. \tag{3.112}$$

Taking into account (3.112) and the integral $\int_0^\infty \left(\mathrm{e}^{-sz} - 1\right)\frac{1}{z}\mathrm{e}^{-\beta z}\mathrm{d}z = -\ln(\frac{s+\beta}{\beta})$, we obtain

$$\mathbb{E}\left\{\mathrm{e}^{-sX_\Gamma(t)}\right\} = \left(\frac{\beta}{s+\beta}\right)^{\gamma_0 t}. \tag{3.113}$$

The expression $\left[\beta/(s+\beta)\right]^{\gamma_0 t}$ is the Laplace transform of the density of the Gamma process [15]. Therefore, we can find an explicit expression for the mesoscopic density of particles for $x \geq 0$:

$$\rho(x,t) = \frac{\partial}{\partial x}\mathbb{P}(X_\Gamma(t) \leq x) = \frac{1}{\Gamma(\gamma_0 t)}\beta^{\gamma_0 t}x^{\gamma_0 t-1}\mathrm{e}^{-\beta x}. \tag{3.114}$$

Since the Lévy measure ν is infinite, i.e., $\nu(\mathrm{d}z) = (\gamma_0/z)\exp(-\beta z)\mathrm{d}z$ is not integrable as $z \to 0$, an infinite number of jumps occurs during a finite period of time. However, the Lévy measure ν can be approximated by

$$\nu_\delta(\mathrm{d}z) = \begin{cases} 0, & z \leq \delta, \\ \left(\gamma_0/z\right)\exp(-\beta z)\mathrm{d}z, & z > \delta, \end{cases} \tag{3.115}$$

where δ is a small number. Introducing the normalization constant $\lambda_\delta = \int_\delta^\infty(\gamma_0/z)$ $\exp(-\beta z)\mathrm{d}z$, we approximate the Gamma process by the compound Poisson process with intensity λ_δ that tends to infinity as $\delta \to 0$. In the limit we have an infinite number of jumps whose size distribution is given by

$$w_\delta(z) = \frac{\left(\gamma_0/z\right)\mathrm{e}^{-\beta z}}{\int_\delta^\infty\left(\gamma_0/z\right)\mathrm{e}^{-\beta z}\mathrm{d}z}. \tag{3.116}$$

The mesoscopic density of particles obeys the integro-differential equation

$$\frac{\partial\rho}{\partial t} = \lambda_\delta\int_0^\infty \rho(x-z,t)w_\delta(z)\mathrm{d}z - \lambda_\delta\rho(x,t). \tag{3.117}$$

3.4 Non-Markovian CTRW Models with Chemical Reactions

In this section we consider CTRW models for which the waiting time distribution is not exponential. The main challenge is to incorporate nonlinear kinetic terms into non-Markovian transport equations. Several approaches exist in the literature about how to include kinetic terms in reaction–transport systems with anomalous diffusion. We discuss them in detail in the following.

We consider a one-component reaction–transport system consisting of particles that follow a CTRW. Let $\rho(x,t)$ represent the density of these particles at point x and time t. We write the reaction term in the form $F(\rho) = f(\rho)\rho$. It is also convenient to represent the nonlinear reaction rate $f(\rho)$ as the difference between the birth rate $f^+(\rho)$ and the death rate $f^-(\rho)$:

$$f(\rho) = f^+(\rho) - f^-(\rho). \tag{3.118}$$

For example, if we consider the Schlögl Model I, see (1.66), then

$$f^+(\rho) = k_1\rho_a, \quad f^-(\rho) = k_3\rho_b + k_2\rho, \tag{3.119}$$

where the densities ρ_a and ρ_b are constant. Note that the birth rate $f^+(\rho)$ must allow for a constant term in $F(\rho)$, as occurs in the Brusselator, the Lengyel–Epstein model, and many other chemical schemes. In those cases, $f^+(\rho) = k\rho^{-1}$. For KPP kinetics, the birth rate is $f^+(\rho) = r$ and the death rate is $f^-(\rho) = r\rho$. The main purpose is to derive the nonlinear Master equation for the density $\rho(x,t)$ in the form $\partial\rho/\partial t = L\rho$, where the nonlinear evolution operator L has to be determined. We consider three different models for reactions and non-Markovian transport processes.

3.4.1 Model A

Non-Markovian behavior of particles performing a CTRW occurs if the particles are trapped for random times distributed according to a nonexponential distribution. The key question is how the chemical reaction influences the statistical properties of the CTRW. For Model A, we assume that the transport process associated with the CTRW and the chemical reactions are independent. We assume that the waiting time PDF $\phi(t)$ and jump length PDF $w(z)$ are independent and that the chemical reactions do not affect *at all* the waiting time PDF. This case has been considered in a series of papers [416, 143, 144, 187]. The main assumption here is that when particles are trapped, the waiting time is the same for all particles, including *newborn* particles. There are various ways to think about this assumption. In a chemical setting, the context of Sokolov and collaborators' work, the assumption implies that reactive events do not destroy or create particles, as for example in an isomerization reaction. Reactions simply change the state, label, or "color" of the particles. Such reactions are known as color-change reactions in the literature [320, 154, 271]. In

these reactions, the particles themselves survive a reactive event and their waiting time is not changed. In a population biology setting, the assumption implies that the *whole* community of individuals moves after a random time t, elapsed since the arrival of the founding members at site x, to a new site $x + z$.

Since the kinetics is of the form $f(\rho)\rho$, the change in the number of particles, of a given type, between the jumps involves the exponential factor $\exp[\int f(\rho(x, u))\mathrm{d}u]$. To explain this, let us introduce the density of particles $j(x, \tau)$ arriving at point x exactly at time τ. During time interval (τ, t), this density changes as follows:

$$j(x, \tau)\mathrm{e}^{\int_\tau^t f(\rho(x,u))\mathrm{d}u}. \tag{3.120}$$

Let us now incorporate this nonlinear kinetic process into a non-Markovian transport process described by a CTRW. We write the equations for the densities $j(x, t)$ and $\rho(x, t)$ in the following forms:

$$\begin{aligned} j(x, t) = &\int_{\mathbb{R}} \rho_0(x - z)\mathrm{e}^{\int_0^t f(\rho(x-z,u))\mathrm{d}u} w(z)\phi(t)\mathrm{d}z \\ &+ \int_0^t \int_{\mathbb{R}} j(x - z, \tau)\mathrm{e}^{\int_\tau^t f(\rho(x-z,u))\mathrm{d}u} w(z)\phi(t - \tau)\mathrm{d}z\mathrm{d}\tau \end{aligned} \tag{3.121}$$

and

$$\begin{aligned} \rho(x, t) = &\rho_0(x)\mathrm{e}^{\int_0^t f(\rho(x,u))\mathrm{d}u}\Psi(t) \\ &+ \int_0^t j(x, \tau)\mathrm{e}^{\int_\tau^t f(\rho(x,u))\mathrm{d}u}\Psi(t - \tau)\mathrm{d}\tau. \end{aligned} \tag{3.122}$$

We are in position now to derive the Master equation for the density $\rho(x, t)$. Since the balance equations (3.121) and (3.122) are nonlinear, we cannot apply the standard technique of the Fourier–Laplace transforms directly. Instead we differentiate the density $\rho(x, t)$ with respect to time:

$$\begin{aligned} \frac{\partial \rho}{\partial t} = &j(x, t) + f(\rho)\rho - \rho_0(x)\mathrm{e}^{\int_0^t f(\rho(x,u))\mathrm{d}u}\phi(t) \\ &- \int_0^t j(x, \tau)\mathrm{e}^{\int_\tau^t f(\rho(x,u))\mathrm{d}u}\phi(t - \tau)\mathrm{d}\tau. \end{aligned} \tag{3.123}$$

The last two terms can be interpreted as the density of particles $i(x, t)$ leaving the point x exactly at time t:

$$\begin{aligned} i(x, t) = &\rho_0(x)\mathrm{e}^{\int_0^t f(\rho(x,u))\mathrm{d}u}\phi(t) \\ &+ \int_0^t j(x, \tau)\mathrm{e}^{\int_\tau^t f(\rho(x,u))\mathrm{d}u}\phi(t - \tau)\mathrm{d}\tau. \end{aligned} \tag{3.124}$$

It follows from (3.121) and (3.124) that $j(x,t) = \int_{\mathbb{R}} i(x-z,t)w(z)\mathrm{d}z$. Then (3.123) can be rewritten as

$$\frac{\partial \rho}{\partial t} = \int_{\mathbb{R}} i(x-z,t)w(z)\mathrm{d}z - i(x,t) + f(\rho)\rho. \tag{3.125}$$

This equation has a very simple meaning as the balance of particles at point x. The first term on the RHS corresponds to the number of particles arriving at x from different positions $x - z$. The second term represents the rate at which the particles leave the position x. The last term describes the rate of change due to kinetics. Note that a similar equation was used in [416]. The advantage of this equation lies in the fact that we do not need the Fourier transform to obtain a closed equation for the density $\rho(x,t)$. Let us express $i(x,t)$ in terms of $\rho(x,t)$. We divide (3.122) and (3.124) by the factor $\mathrm{e}^{\int_0^t f(\rho(x,u))\mathrm{d}u}$ and take the Laplace transform $\mathcal{L}$ of both equations:

$$\mathcal{L}\left\{\rho(x,t)\mathrm{e}^{-\int_0^t f(\rho(x,u))\mathrm{d}u}\right\} = \left[\rho_0(x) + \mathcal{L}\left\{j(x,t)\mathrm{e}^{-\int_0^t f(\rho(x,u))\mathrm{d}u}\right\}\right]\hat{\Psi}(s), \tag{3.126}$$

$$\mathcal{L}\left\{i(x,t)\mathrm{e}^{-\int_0^t f(\rho(x,u))\mathrm{d}u}\right\} = \left[\rho_0(x) + \mathcal{L}\left\{j(x,t)\mathrm{e}^{-\int_0^t f(\rho(x,u))\mathrm{d}u}\right\}\right]\hat{\phi}(s). \tag{3.127}$$

From these two equations, we obtain

$$\mathcal{L}\left\{i(x,t)\mathrm{e}^{-\int_0^t f(\rho(x,u))\mathrm{d}u}\right\} = \frac{\hat{\phi}(s)}{\hat{\Psi}(s)}\mathcal{L}\left\{\rho(x,t)\mathrm{e}^{-\int_0^t f(\rho(x,u))\mathrm{d}u}\right\}. \tag{3.128}$$

The inverse Laplace transform yields the expression for $i(x,t)$:

$$i(x,t) = \int_0^t K(t-\tau)\rho(x,\tau)\mathrm{e}^{\int_\tau^t f(\rho(x,u))\mathrm{d}u}\mathrm{d}\tau, \tag{3.129}$$

where $K(t)$ is the standard memory kernel (3.34). Substitution of (3.129) into (3.125) results in the Master equation:

$$\begin{aligned}\frac{\partial \rho}{\partial t} = \int_0^t K(t-\tau)\Bigg[\int_{\mathbb{R}} \rho(x-z,\tau)\mathrm{e}^{\int_\tau^t f(\rho(x-z,u))\mathrm{d}u}w(z)\mathrm{d}z \\ -\rho(x,\tau)\mathrm{e}^{\int_\tau^t f(\rho(x,u))\mathrm{d}u}\Bigg]\mathrm{d}\tau + f(\rho)\rho.\end{aligned} \tag{3.130}$$

Now consider the case where the reaction rate $f(\rho) = r = \text{const}$. Then the Master equation takes the form

$$\frac{\partial \rho}{\partial t} = \int_0^t K(t-\tau) \mathrm{e}^{r(t-\tau)} \left[\int_{\mathbb{R}} \rho(x-z,\tau) w(z) \mathrm{d}z - \rho(x,\tau) \right] \mathrm{d}\tau + r\rho. \quad (3.131)$$

It is tempting to claim that this equation describes the coupling of chemical reaction and transport. We believe that this is misleading. In fact, this equation describes the perfect decoupling of transport with memory and linear reaction, in line with the main assumption of Model A. To show this, we make the substitution

$$\rho(x,t) = n(x,t)\mathrm{e}^{rt}. \quad (3.132)$$

Then we obtain the following equation for $n(x,t)$,

$$\frac{\partial n}{\partial t} = \int_0^t K(t-\tau) \left[\int_{\mathbb{R}} n(x-z,\tau) w(z) \mathrm{d}z - n(x,\tau) \right] \mathrm{d}\tau, \quad (3.133)$$

which is independent of the reaction and describes the transport of passive particles. So we have a perfect decoupling for which the density $\rho(x,t)$ is the product of the density of passive particles $n(x,t)$ and the exponential factor e^{rt} due to reaction.

3.4.2 Model B

This model is equivalent to the Vlad–Ross approach of Sect. 2.3.2. We consider a CTRW which depends on the chemical reaction in the following way. Assume that the particles that are created with the rate $f^+(\rho)\rho$ have zero age. Note that particles also have zero age when they just arrive at some point x from which they will jump later. We interpret the density $j(x,t)$ as a zero-age density of particles arriving at the point x exactly at time t due to a jump process or a birth process with the rate $f^+(\rho)$. Equations for the densities $j(x,t)$ and $\rho(x,t)$ can be written as

$$\begin{aligned} j(x,t) = f^+(\rho)\rho &+ \int_{\mathbb{R}} \rho_0(x-z) \mathrm{e}^{-\int_0^t f^-(\rho(x-z,u))\mathrm{d}u} w(z)\phi(t)\mathrm{d}z \\ &+ \int_0^t \int_{\mathbb{R}} j(x-z,\tau) \mathrm{e}^{-\int_\tau^t f^-(\rho(x-z,u))\mathrm{d}u} w(z)\phi(t-\tau)\mathrm{d}z\mathrm{d}\tau \end{aligned} \quad (3.134)$$

and

$$\begin{aligned} \rho(x,t) = \rho_0(x) &\mathrm{e}^{-\int_0^t f^-(\rho(x,u))\mathrm{d}u} \Psi(t) \\ &+ \int_0^t j(x,\tau) \mathrm{e}^{-\int_\tau^t f^-(\rho(x,u))\mathrm{d}u} \Psi(t-\tau)\mathrm{d}\tau. \end{aligned} \quad (3.135)$$

A single equation for the density $\rho(x,t)$ can be derived in the same way as for Model A. It takes the form

$$\frac{\partial \rho}{\partial t} = \int_0^t K(t-\tau)\Bigg[\int_{\mathbb{R}} \rho(x-z,\tau)\mathrm{e}^{-\int_\tau^t f^-(\rho(x-z,u))\mathrm{d}u} w(z)\mathrm{d}z \\ -\rho(x,\tau)\mathrm{e}^{-\int_\tau^t f^-(\rho(x,u))\mathrm{d}u}\Bigg]\mathrm{d}\tau + f^+(\rho)\rho - f^-(\rho)\rho. \tag{3.136}$$

If we expand the expression in brackets for small z and truncate the Taylor series at the second moment, we obtain

$$\frac{\partial \rho}{\partial t} = \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}\int_0^t K(t-\tau)\rho(x,\tau)\mathrm{e}^{-\int_\tau^t f^-(\rho(x,u))\mathrm{d}u}\mathrm{d}\tau \\ +f^+(\rho)\rho - f^-(\rho)\rho, \tag{3.137}$$

which is identical with (2.82). Model B describes the situation where reactant particles are destroyed and product particles are created during a reactive event, the common situation in a chemical context, and where consequently the newborn product particles are endowed a new waiting time. This model does not distinguish between arrival of a particle at site x by reaction (birth) or by transport (jump); it treats both processes on the same footing. Model B is expected to describe chemical reactions in static porous or disordered media. Age on page 82 refers to the waiting time of particles at a given point. Note that we do not consider aging effects of the system as stated on page 64.

Models A and B result in the same reaction–transport equation, if the CTRW is Markovian. In that case, $K(t-\tau) = \delta(t-\tau)/\tau_0$, see Remark 2.5, and the Master equations (3.130) and (3.136) are identical:

$$\frac{\partial \rho}{\partial t} = \frac{1}{\tau_0}\Bigg[\int_{\mathbb{R}} \rho(x-z,t)w(z)\mathrm{d}z - \rho(x,t)\Bigg] + f(\rho)\rho. \tag{3.138}$$

3.4.3 Model C

This is a very simple model. It assumes that the reaction is a pure birth process. It corresponds to the case where the reaction term is $F(\rho) = f^+(\rho)\rho$. This model was considered in [188, 189, 121]. The balance equations are

$$j(x,t) = f^+(\rho)\rho + \int_{\mathbb{R}} \rho_0(x-z)\psi(z,t)\mathrm{d}z \\ +\int_0^t\int_{\mathbb{R}} j(x-z,t-\tau)\psi(z,\tau)\mathrm{d}z\mathrm{d}\tau \tag{3.139}$$

and

$$\rho(x,t) = \rho_0(x)\Psi(t) + \int_0^t j(x,t-\tau)\Psi(\tau)\mathrm{d}\tau. \tag{3.140}$$

This system of equations can be written as a single equation for the density

$$\rho(x,t) = \rho_0(x)\Psi(t) + \int_0^t \int_{\mathbb{R}} \rho(x-z, t-\tau)\psi(z,\tau)\mathrm{d}z\mathrm{d}\tau + \int_0^t f^+(\rho(x,t-\tau))\rho(x,t-\tau)\Psi(\tau)\mathrm{d}\tau. \tag{3.141}$$

Thus the simplest way to take into account the chemical reaction is to add the term $\int_0^t F(\rho(x,t-\tau))\Psi(\tau)\mathrm{d}\tau$ to the RHS of the balance equation (3.41). The reaction term $F(\rho) = f^+(\rho)\rho$ is a pure birth process for which all newborn particles are given zero age.

Equation (3.141) takes the following form in Fourier–Laplace space:

$$\hat{\tilde{\rho}}(k,s) = \tilde{\rho}_0(k)\hat{\Psi}(s) + \hat{\tilde{\rho}}(k,s)\hat{\tilde{\psi}}(k,s) + \hat{\tilde{F}}(k,s)\hat{\Psi}(s). \tag{3.142}$$

We assume that the random jumps and the waiting times are independent, i.e., $\hat{\tilde{\psi}}(k,s) = \tilde{w}(k)\hat{\phi}(s)$, and divide (3.142) by $\hat{\phi}(s)$ to separate temporal and spatial variables:

$$\frac{\hat{\tilde{\rho}}(k,s)}{\hat{\phi}(s)} - \frac{\tilde{\rho}_0(k)\hat{\Psi}(s)}{\hat{\phi}(s)} = \hat{\tilde{\rho}}(k,s)\tilde{w}(k) + \frac{\hat{\tilde{F}}(k,s)\hat{\Psi}(s)}{\hat{\phi}(s)}. \tag{3.143}$$

If the waiting time PDF and the jump length PDF do not possess heavy tails, then the mean waiting time and the variance of the jump length PDF are finite, and we have the following results in the large-time and large-scale limit, see Sect. 3.2. First, the Fourier transform of the even dispersal kernel can be written as

$$\tilde{w}(k) = 1 - \sigma^2 k^2/2 + o(k^2), \tag{3.144}$$

since

$$\tilde{w}(0) = \int_{-\infty}^{\infty} w(x)\mathrm{d}x = 1, \quad \tilde{w}'(0) = 0, \quad \sigma^2 = -\tilde{w}''(0) = \int_{-\infty}^{\infty} x^2 w(x)\mathrm{d}x. \tag{3.145}$$

Second, $1/\hat{\phi}(s)$ can be written as

$$\frac{1}{\hat{\phi}(s)} \simeq 1 + \langle t\rangle s, \tag{3.146}$$

up to first order in s, or

$$\frac{1}{\hat{\phi}(s)} \simeq 1 + \langle t\rangle s + \left(\langle t\rangle^2 - \frac{\langle t^2\rangle}{2}\right)s^2 \tag{3.147}$$

up to second order, since

$$\hat{\phi}(0) = \int_0^\infty \phi(t)\mathrm{d}t = 1, \quad \langle t\rangle = -\hat{\phi}'(0) = \int_0^\infty t\phi(t)\mathrm{d}t, \tag{3.148}$$

$$\langle t^2\rangle = \hat{\phi}''(0) = \int_0^\infty t^2\phi(t)\mathrm{d}t. \tag{3.149}$$

Substituting (3.144) into (3.143) and using that $\hat{\Psi}(s) = [1-\hat{\phi}(s)]/s$, we obtain

$$\frac{1-\hat{\phi}(s)}{\hat{\phi}(s)}\left[\hat{\tilde{\rho}}(k,s) - \frac{\tilde{\rho}(k,0)}{s}\right] = -\frac{\sigma^2k^2}{2}\hat{\tilde{\rho}}(k,s) + \frac{1-\hat{\phi}(s)}{s\hat{\phi}(s)}\hat{\tilde{F}}(k,s). \tag{3.150}$$

Substitution of (3.146) into (3.150) and inversion of the Fourier and Laplace transforms leads to the RD equation (2.3) with $D = \sigma^2/2\langle t\rangle$. If we substitute (3.147) into (3.150) and invert the Fourier and Laplace transforms, we obtain the reaction-telegraph equation:

$$\left(\langle t\rangle - \frac{\langle t^2\rangle}{2\langle t\rangle}\right)\frac{\partial^2\rho}{\partial t^2} + \frac{\partial\rho}{\partial t} = \frac{\sigma^2}{2\langle t\rangle}\frac{\partial^2\rho}{\partial x^2} + F + \left(\langle t\rangle - \frac{\langle t^2\rangle}{2\langle t\rangle}\right)\frac{\partial F}{\partial t}. \tag{3.151}$$

A comparison of (2.19) and (3.151) leads to the relation between the macroscopic parameters τ (relaxation time) and D (diffusion coefficient) and the mesoscopic quantities, namely

$$\tau = \langle t\rangle - \frac{\langle t^2\rangle}{2\langle t\rangle} \quad \text{and} \quad D = \frac{\sigma^2}{2\langle t\rangle}. \tag{3.152}$$

3.5 Random Walk in Random Time and Subordination

In this section we consider a random walk in random time. In this case the particle position X depends on the random time $T(t)$, $X(T(t))$, rather than on the conventional time t. An insight into this model can be obtained by considering a particle moving in a nonstationary random environment for which the intensity of jumps is random. We use the standard formula for the particle position as the sum of IID random jumps Z_i,

$$X(t) = \sum_{i=1}^{N(t)} Z_i, \tag{3.153}$$

in which the number of jumps $N(t)$ is a nonhomogeneous Poisson process with the random intensity $\lambda(t) \geq 0$. For example, one can think of a particle moving in a random turbulent flow. The process $X(t)$ is called a *compound Cox process* and $N(t)$ is a *doubly stochastic Poisson process*. The probability of n jumps up to time t is

$$\mathbb{P}(N(t)=n)=\mathbb{E}_{\lambda}\left\{\frac{\left(\int_0^t\lambda(s)\mathrm{d}s\right)^n}{n!}\exp\left(-\int_0^t\lambda(s)\mathrm{d}s\right)\right\}, \tag{3.154}$$

where the expectation $\mathbb{E}_{\lambda}$ is taken over the random process $\lambda(t)$. If we introduce the random time $T(t)=\lambda^{-1}\int_0^t\lambda(s)\mathrm{d}s$, then the Cox process $N(t)$ can be rewritten in terms of a homogeneous Poisson process $N_h(t)$ with intensity λ and random time $T(t)$ as

$$N(t)=N_h(T(t)). \tag{3.155}$$

It follows from (3.153) and (3.155) that the particle position depends on $T(t)$:

$$X(T(t))=\sum_{i=1}^{N_h(T(t))}Z_i. \tag{3.156}$$

In what follows we put the intensity of the Poisson process $\lambda=1$ and treat both t and $T(t)$ as dimensionless.

Let us now consider the random time $T(t)$ which is assumed to have nonnegative stationary and independent increments, an increasing Lévy process, such that $T(t)\geq 0$, $T(0)=0$, and $T(t)\leq T(s)$ whenever $t\leq s$. It is often referred to as a *subordinator* or *operational time* (we assume that $T(t)$ and $N_h(t)$ are independent). If $X(t)$ is a Markov process, then the process $X(T(t))$ is Markovian too. The later process is said to be subordinate to $X(t)$ [15, 126].

Our goal is to find an equation for the density of particles that follow the random walk (3.156). First, let us find the characteristic function

$$\tilde{\rho}(k,t)=\mathbb{E}\left(\mathrm{e}^{\mathrm{i}kX(t)}\right)=\sum_{n=0}^{\infty}\mathbb{E}\left(\mathrm{e}^{\mathrm{i}kX(t)}\big|N(t)=n\right)\mathbb{P}(N(t)=n). \tag{3.157}$$

Recall that we interpret this function as the Fourier transform of the density $\rho(x,t)$ with $\rho(x,0)=\delta(x)$. The conditional expectation is given by $\mathbb{E}\left(\mathrm{e}^{\mathrm{i}kX(t)}\big|N(t)=n\right)=\tilde{w}^n(k)$, where $\tilde{w}(k)=\mathbb{E}\left(\mathrm{e}^{\mathrm{i}kZ_i}\right)$ is the characteristic function of the random jumps Z_i. Using $N(t)=N_h(T(t))$ with $\lambda=1$, we find

$$\mathbb{P}(N(t)=n)=\int_0^{\infty}\mathbb{P}(N_h(\tau)=n)p_T(\tau,t)\mathrm{d}\tau=\int_0^{\infty}\frac{\tau^n\mathrm{e}^{-\tau}}{n!}p_T(\tau,t)\mathrm{d}\tau, \tag{3.158}$$

where $p_T(\tau,t)$ is the PDF of the random time $T(t)$, defined as

$$p_T(\tau,t)=\frac{\partial}{\partial\tau}\mathbb{P}(T(t)\leq\tau). \tag{3.159}$$

Substitution of (3.158) into (3.157) yields

$$\tilde{\rho}(k,t) = \sum_{n=0}^{\infty} \int_0^{\infty} \tilde{w}^n(k) \frac{(\tau)^n \mathrm{e}^{-\tau}}{n!} p_T(\tau,t)\mathrm{d}\tau$$
$$= \int_0^{\infty} \mathrm{e}^{\tau(\tilde{w}(k)-1)} p_T(\tau,t)\mathrm{d}\tau = \mathbb{E}\left(\mathrm{e}^{T(t)(\tilde{w}(k)-1)}\right). \tag{3.160}$$

Since $T(t) \geq 0$ is a Lévy process, its Laplace transform, the moment generating function can be written as

$$\mathbb{E}\left(\mathrm{e}^{-sT(t)}\right) = \mathrm{e}^{-tl(s)}, \tag{3.161}$$

where $l(s)$ is the Laplace exponent of the random time $T(t)$. Using (3.160) and (3.161), we obtain

$$\tilde{\rho}(k,t) = \mathrm{e}^{-tl(-(\tilde{w}(k)-1))}. \tag{3.162}$$

This implies that the characteristic exponent $\psi(k)$ for the particle position $X(t)$ is

$$\psi(k) = -l(-(\tilde{w}(k)-1)). \tag{3.163}$$

For example, if the random time $T(t)$ is the Poisson process $N(t)$ with $\lambda = 1$, then the Laplace transform $\mathbb{E}\left(\mathrm{e}^{-sN(t)}\right) = \sum_{n=0}^{\infty} \mathrm{e}^{-sn}\mathbb{P}(N(t)=n) = \mathrm{e}^{-t\left(1-\mathrm{e}^{-s}\right)}$, therefore $l(s) = \left(1-\mathrm{e}^{-s}\right)$. In the long-time limit, $l(s) = s + o(s)$ as $s \to 0$. This limit corresponds to the Kolmogorov–Feller equation.

It follows from (3.89) that the mesoscopic transport equation for the density of particles is

$$\frac{\partial \rho}{\partial t} = L\rho, \tag{3.164}$$

where L is a pseudo-differential operator with symbol given by (3.163), $\mathcal{F}[L\rho] = \psi(k)\tilde{\rho}(k,t)$. When the random time $T(t)$ is deterministic $T(t) = t$, then the Laplace exponent is $l(s) = s$, the characteristic exponent defined in (3.161) is $\psi(k) = \tilde{w}(k) - 1$ and Eq. (3.164) becomes the Kolmogorov–Feller equation.

3.5.1 Space-Fractional Transport Equation

In this section we use the idea of subordination to obtain the space-fractional transport equation. Since $T(t)$ is a nonnegative Lévy process, the Laplace exponent $l(s)$ defined in (3.161) can be written as

$$l(s) = as + \int_0^{\infty} \left(1 - \mathrm{e}^{-sz}\right) \nu(\mathrm{d}z), \tag{3.165}$$

where $a \geq 0$ and $\nu(A) \geq 0$ is a Lévy measure satisfying $\int_{(0,\infty)} \min(1, z)\nu(\mathrm{d}z) < \infty$ [15].

γ-stable subordinator. As an example, consider a strictly γ-stable random time $T_\gamma(t)$, the stable subordinator, for which $a = 0$ and the Lévy measure is

$$\nu(\mathrm{d}z) = \frac{\gamma \mathrm{d}z}{\Gamma(1-\gamma)z^{1+\gamma}} \tag{3.166}$$

with $0 < \gamma < 1$. Let us find the Laplace exponent $l(s)$ of the γ-stable random time $T_\gamma(t)$. Integration by parts in (3.165) shows that $l(s) = s^\gamma$. Thus

$$\mathbb{E}\left(\mathrm{e}^{-sT_\gamma(t)}\right) = \int_0^\infty \mathrm{e}^{-s\tau} p_T(\tau, t)\mathrm{d}\tau = \mathrm{e}^{-ts^\gamma}, \tag{3.167}$$

which implies that $\mathbb{E}\left[T_\gamma(t)\right] = \infty$. The PDF $p_T(\tau, t)$ can be written in terms of the strictly γ-stable PDF $g_\gamma(\tau)$ with the Laplace transform

$$\hat{g}_\gamma(s) = \mathrm{e}^{-s^\gamma}, \ 0 < \gamma < 1. \tag{3.168}$$

The strictly stable process $T_\gamma(t)$ has a nice scaling property: $T_\gamma(t) \stackrel{d}{=} t^{1/\gamma} T_\gamma(1)$ for all t. Scaling arguments lead to

$$p_T(\tau, t) = \frac{1}{t^{1/\gamma}} g_\gamma\left(\tau/t^{1/\gamma}\right). \tag{3.169}$$

Since the asymptotic decay of the tail of $g_\gamma(\tau)$ is $\tau^{-(1+\gamma)}$ as $\tau \to \infty$, we conclude that $p_T(\tau, t)$ has a power-law tail

$$p_T(\tau, t) \sim \frac{t}{\tau^{1+\gamma}} \tag{3.170}$$

as $\tau \to \infty$. The density $p_T(\tau, t)$ admits an explicit representation for $\gamma = \frac{1}{2}$ in terms of the Lévy–Smirnov density $g_{1/2}(\tau) = \left(4\pi\tau^3\right)^{-1/2} \exp(-1/4\tau)$:

$$p_T(\tau, t) = t^{-2} g_{1/2}\left(\tau/t^2\right) = \frac{t}{2\sqrt{\pi\tau^3}} \exp\left(-\frac{t^2}{4\tau}\right). \tag{3.171}$$

It follows from (3.163) that $\psi(k) = -[-(\tilde{w}(k) - 1)]^\gamma$. The governing equation for the particle density is the mesoscopic transport equation

$$\frac{\partial \rho}{\partial t} = \mathcal{I}_\gamma \rho(x, t), \tag{3.172}$$

where the right-hand side is the fractional integral operator, defined as

$$\mathcal{I}_\gamma g(x) = \mathcal{F}^{-1}\left[-(-(\tilde{w}(k) - 1))^\gamma \tilde{g}(k)\right], \tag{3.173}$$

and $\mathcal{F}^{-1}$ denotes the inverse Fourier transform. This operator can be considered as a generalization of the fractional Laplace operator. In the large-scale limit, $\tilde{w}(k)-1 = -\sigma^2 k^2/2 + o(k^2)$ as $k \to 0$, the transport equation (3.172) can be approximated by the standard space-fractional diffusion equation

$$\frac{\partial \rho}{\partial t} = \frac{\sigma^\alpha}{\sqrt{2^\alpha}} \frac{\partial^\alpha \rho}{\partial |x|^\alpha} \tag{3.174}$$

with $\alpha = 2\gamma$.

If the density of particles following the Lévy process $X(t)$ is $\rho_X(x,t)$, then the density of particles performing the random walk $Y(t) = X(T(t))$ can be defined as

$$\rho_Y(x,t) = \int_0^\infty \rho_X(x,\tau) p_T(\tau,t) \mathrm{d}\tau, \tag{3.175}$$

where $p_T(\tau,t) = \frac{\partial}{\partial \tau}\mathbb{P}(T(t) \le \tau)$ is the density of the random time $T(t)$. Note that the random process $Y(t)$ is a Lévy process too. In order to illustrate how the formula can be used, we consider the particles following the diffusion process $X(t)$ for which

$$\rho_X(x,\tau) = \frac{1}{\sqrt{2\pi\sigma^2\tau}} \exp\left(-\frac{x^2}{2\sigma^2\tau}\right). \tag{3.176}$$

Substitution of (3.176) and (3.171) into (3.175) yields the Cauchy density

$$\rho_Y(x,t) = \frac{\sigma t}{\sqrt{2}\pi\left(x^2 + \sigma^2 t^2/2\right)}. \tag{3.177}$$

This density is the Green function for the space-fractional equation (3.174) with $\alpha = 1$. The characteristic exponent $\psi_Y(k)$ of the new process $Y(t)$ can be obtained as a composition of the Laplace exponent $l(s)$ with the characteristic exponent $\psi_X(k)$, i.e.,

$$\mathbb{E}\left\{\mathrm{e}^{\mathrm{i}kY(t)}\right\} = \mathrm{e}^{-t\psi_Y(k)} = \mathrm{e}^{-tl(-\psi_X(k))}. \tag{3.178}$$

We find

$$\begin{aligned}\mathbb{E}\left\{\mathrm{e}^{\mathrm{i}kY(t)}\right\} &= \int_0^\infty \mathbb{E}\left\{\mathrm{e}^{\mathrm{i}kX(T(s))}\right\} p_T(s,t)\mathrm{d}s \\ &= \int_0^\infty \mathrm{e}^{T(s)\psi_X(k)} p_T(s,t)\mathrm{d}s = \mathrm{e}^{-tl(-\psi_X(k))}.\end{aligned} \tag{3.179}$$

Hougaard subordinator (tempered stable subordinator). Another example of a random time is the Hougaard subordinator $T(t)$ with the Lévy measure

$$\nu(\mathrm{d}z) = \frac{\gamma\xi \mathrm{e}^{-kz}}{\Gamma(1-\gamma)z^{1+\gamma}}\mathrm{d}z, \quad z > 0, \tag{3.180}$$

where $k \geq 0, \xi > 0$, and $0 < \gamma < 1$. This density is obtained from the γ-stable density if we multiply it by the factor $\xi \mathrm{e}^{-kz}$. The Laplace transform for the Hougaard process is

$$\mathbb{E}\left\{\mathrm{e}^{-sT(t)}\right\} = \exp\left[t\int_0^\infty (1-\mathrm{e}^{-sz})\nu(\mathrm{d}z)\right] = \mathrm{e}^{-t\xi\left[(k+s)^\gamma - k^\gamma\right]}, \quad s \geq 0. \tag{3.181}$$

The Laplace exponent is $l(s) = \xi\left[(k+s)^\gamma - k^\gamma\right]$. For $\gamma = 1$ we have a deterministic process $T(t) = \xi t$. If $k = 0$ and $\xi = 1$ we have a γ-stable subordinator. In particular, the mean value is

$$\mathbb{E}\{T(t)\} = -\frac{\partial}{\partial s}\mathbb{E}\left\{\mathrm{e}^{-sT(t)}\right\}_{s=0} = \frac{\gamma\xi t}{k^{1-\gamma}} \tag{3.182}$$

and it is finite. It is clear that $\mathbb{E}\{T(t)\} \to \infty$ as $k \to 0$ for $0 < \gamma < 1$. So the Hougaard subordinator is useful when we consider transport processes with both normal and anomalous behaviour.

3.5.2 Inverse Subordination and Time-Fractional Transport Equation

In this section we show how to obtain subdiffusive transport by using the idea of inverse subordination [278, 371]. Assume that the density $\rho_X(x,t)$ obeys the Kolmogorov–Feller equation

$$\frac{\partial \rho_X}{\partial t} = \int_{\mathbb{R}} \rho_X(x-z,t)w(z)\mathrm{d}z - \rho_X(x,t) \tag{3.183}$$

with the initial condition

$$\rho_X(x,0) = \rho_0(x). \tag{3.184}$$

We define the particle density $\rho(x,t)$ as follows:

$$\rho(x,t) = \int_0^\infty \rho_X\left(x, \left(\frac{t}{\tau}\right)^\gamma\right) g_\gamma(\tau)\mathrm{d}\tau, \tag{3.185}$$

where $g_\gamma(\tau)$ is the density of the γ-stable variable with $0 < \gamma < 1$ defined by the Laplace transform (3.168). Then $\rho(x,t)$ satisfies the time-fractional Kolmogorov–Feller equation

$$\frac{\partial^\gamma \rho}{\partial t^\gamma} = \int_{\mathbb{R}} \rho(x-z,t)w(z)\mathrm{d}z - \rho(x,t), \tag{3.186}$$

where $\partial^\gamma \rho / \partial t^\gamma$ is the Caputo fractional derivative and time t is dimensionless. The main idea here is the introduction of the subordinated process, the position of particles $X(N_\gamma(t))$, whose mesoscopic density is $\rho(x,t)$. The parent process $X(t)$ is the compound Poisson process with the density $\rho_X(x,t)$ and the random time $N_\gamma(t)$ is the inverse γ-stable subordinator defined as the hitting time $N_\gamma(t) = \inf(\tau : T_\gamma(\tau) > t)$ for γ-stable subordinator $T_\gamma(\tau)$ with the Laplace exponent $l(s) = s^\gamma$. The non-Markovian behavior of the inverse subordinator $N_\gamma(t)$ leads to subdiffusion of $X(N_\gamma(t))$. The details of the derivation of (3.186) can be found in [278]. Note that as the parent process $X(t)$ one can use any Lévy process with the transport operator L, so the time-fractional equation is of the form $\partial^\gamma \rho / \partial t^\gamma = L\rho$.

3.6 Macroscopic Description

The term *macroscopic* description refers to the long-time and large-scale limit, $t \to \infty$ and $x \to \infty$, of mesoscopic equations where the details of the *microscopic* movement are irrelevant. In particular, it refers to the *diffusive limit* where balance equations such as (3.13), (3.41), and (3.74) are approximated by the diffusion equation (2.1). The standard derivation of the diffusion equation involves the assumption that the typical microscopic jumps and times are small compared to the characteristic macroscopic space and time scales. Let us illustrate this using the mesoscopic transport equation (3.74). If the jump density $w(z)$ is a rapidly decaying function for large z, one can expand $\rho(x - z, t)$ in z and truncate the Taylor series at the second moment:

$$\rho(x - z, t) = \rho(x, t) - \frac{\partial \rho}{\partial x} z + \frac{1}{2} \frac{\partial^2 \rho}{\partial x^2} z^2 + o(z^2). \tag{3.187}$$

Substitution of (3.187) into (3.74) yields

$$\frac{\partial \rho}{\partial t} + v \frac{\partial \rho}{\partial x} = D \frac{\partial^2 \rho}{\partial x^2}, \tag{3.188}$$

where

$$v = \lambda \int_{\mathbb{R}} z w(z) \mathrm{d}z, \quad D = \frac{\lambda}{2} \int_{\mathbb{R}} z^2 w(z) \mathrm{d}z. \tag{3.189}$$

This truncation is a well-defined procedure, if the higher moments become progressively smaller. If the jump density $w(z)$ is even, then we obtain the standard diffusion equation. However, this "naive" Taylor series expansion is not valid for "heavy-tailed" probability density functions, such as a Cauchy PDF,

$$w(z) = \frac{\sigma}{\pi \left(\sigma^2 + z^2 \right)}, \tag{3.190}$$

for which the second moment, $\int_{\mathbb{R}} z^2 w(z)\mathrm{d}z$, diverges. A jump PDF is said to have a power-law tail if

$$w(z) \sim \frac{1}{|z|^{1+\alpha}}, \quad z \to \infty, \tag{3.191}$$

for which the nth moment exists if $n < \alpha$. The question arises for which values of the power-law exponent α the diffusion approximation (2.1) is not valid.

3.6.1 Scaling Procedure

In this section we use a scaling procedure to derive *macroscopic* equation. This allows us to understand the connection between *macroscopic* and *microscopic* descriptions. We introduce the *macroscopic* variables (x^*, t^*) as follows:

$$x^* = \varepsilon^H x, \quad t^* = \varepsilon t, \tag{3.192}$$

where ε is a small parameter and H is a scaling exponent that has to be determined. It is convenient to introduce such a small parameter, so that instead of taking the limits $t \to \infty$ and $x \to \infty$, we can consider $\varepsilon \to 0$ for fixed values of the *macroscopic* space–time variables (x^*, t^*). We now drop the asterisk for *macroscopic* variables and adopt the following notation for rescaling:

$$x \to \frac{x}{\varepsilon^H}, \quad t \to \frac{t}{\varepsilon}. \tag{3.193}$$

To illustrate the method, we derive the diffusion equation corresponding to the discrete balance equation (3.13). For simplicity, we assume that the jump density is an even function, $w(z) = w(-z)$. We introduce the continuous-time variable t so that $n = [t]$, where $[\cdot]$ denotes the integer part of a real number. Using (3.193), we obtain the rescaled density

$$\rho^\varepsilon(x, t) = \rho\left(\frac{x}{\varepsilon^H}, \left[\frac{t}{\varepsilon}\right]\right). \tag{3.194}$$

Note that $[t/\varepsilon] \approx t/\varepsilon$ as $\varepsilon \to 0$. From (3.13) we obtain the equation

$$\rho^\varepsilon(x, t+\varepsilon) = \int_{\mathbb{R}} \rho^\varepsilon\left(x - \varepsilon^H z, t\right) w(z)\mathrm{d}z. \tag{3.195}$$

It is clear that after rescaling the time step, $\varepsilon \ll 1$, the jump size is proportional to ε^H. In the limit $\varepsilon \to 0$, we expand both sides of the rescaled equation (3.195) in a Taylor series as

$$\rho^{\varepsilon}(x,t)+\frac{\partial\rho^{\varepsilon}}{\partial t}\varepsilon+o(\varepsilon)=\rho^{\varepsilon}(x,t)+\frac{\sigma^2}{2}\frac{\partial^2\rho^{\varepsilon}}{\partial x^2}\varepsilon^{2H}+o\left(\varepsilon^{2H}\right), \tag{3.196}$$

where $\sigma^2=\int_{\mathbb{R}}z^2w(z)\mathrm{d}z$. To obtain the *macroscopic* diffusion equation for the density $\rho(x,t)=\lim_{\varepsilon\to 0}\rho^{\varepsilon}(x,t)$, we must choose $H=1/2$. Then (3.196) turns into (2.1) with the diffusion coefficient $D=\sigma^2/2$. This limit has a very nice probabilistic interpretation. First let us consider the discrete case. It follows from the central limit theorem (CLT) that if the number of steps n is large, the rescaled particle position $X_n/n^{\frac{1}{2}}$ tends to a Gaussian variable with zero mean and variance σ^2. The random position X_n is defined in (3.10). In particular $\mathbb{E}X_n^2=\sigma^2 n$. The functional CLT states that if Z_i is a sequence of IID random variables with zero mean and variance $\sigma^2=\mathbb{E}\left(Z_i^2\right)$, then

$$\frac{X_{[nt]}}{n^{\frac{1}{2}}}=\frac{1}{n^{\frac{1}{2}}}\sum_{i=1}^{[nt]}Z_i\xrightarrow{\mathrm{d}}B(t)\text{ as }n\to\infty, \tag{3.197}$$

where $\xrightarrow{\mathrm{d}}$ means convergence in distribution. Here $B(t)$ is the Brownian motion with the PDF

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathbb{P}(B(t)\le x)=\frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right), \tag{3.198}$$

which is the Green's function for the diffusion equation (2.1) with $D=\sigma^2/2$.

Using the rescaling $t\to t/\varepsilon$ with a small parameter $\varepsilon=n^{-1}$ and fixed time t, we write a rescaled particle position $X^{\varepsilon}(t)$ in terms of X_n:

$$X^{\varepsilon}(t)=\varepsilon^{\frac{1}{2}}X_{[t/\varepsilon]}=\varepsilon^{\frac{1}{2}}\sum_{i=1}^{[t/\varepsilon]}Z_i. \tag{3.199}$$

The functional CLT ensures that as $\varepsilon\to 0$, the random process $X^{\varepsilon}(t)$ converges to the Brownian motion $B(t)$. The PDF $p^{\varepsilon}(x,t)$ for the particle position $X^{\varepsilon}(t)$, starting at $x=0$, satisfies

$$\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}p^{\varepsilon}(x,t)=\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}p\left(\frac{x}{\varepsilon^{\frac{1}{2}}},\left[\frac{t}{\varepsilon}\right]\right)=\frac{1}{\sqrt{2\pi\sigma^2 t}}\left(-\frac{x^2}{2\sigma^2 t}\right) \tag{3.200}$$

where $p(x,t)$ is defined in (3.11).

It is instructive to show that $X^{\varepsilon}(t)\xrightarrow{\mathrm{d}}B(t)$ as $\varepsilon\to 0$. Let us use the characteristic function

$$\mathbb{E}\left\{\exp(\mathrm{i}kX^{\varepsilon}(t))\right\} = \mathbb{E}\left\{\exp\left(\mathrm{i}k\varepsilon^{\frac{1}{2}}\sum_{i=1}^{[t/\varepsilon]} Z_i\right)\right\} = \left(\mathbb{E}\left\{\exp\left(\mathrm{i}k\varepsilon^{\frac{1}{2}}Z_i\right)\right\}\right)^{[t/\varepsilon]}. \tag{3.201}$$

In the limit $\varepsilon \to 0$, we have $[t/\varepsilon] \approx t/\varepsilon$, and $\mathbb{E}\left\{\exp(\mathrm{i}kX^{\varepsilon}(t))\right\} = (1 - k^2\varepsilon\sigma^2/2 + o(\varepsilon))^{t/\varepsilon} \to \exp(-k^2\sigma^2 t/2)$. That is

$$\lim_{\varepsilon\to 0}\mathbb{E}\left\{\exp\left(\mathrm{i}kX^{\varepsilon}(t)\right)\right\} = \exp\left(-Dk^2 t\right), \tag{3.202}$$

which is a characteristic function of the Brownian motion with $D = \sigma^2/2$. In the next section we consider the case where the random variables Z_i have infinite second moments, which leads to the anomalous scaling $x \to x/\varepsilon^{1/\alpha}$, $t \to t/\varepsilon$, and $\lim_{\varepsilon\to 0}\mathbb{E}\left\{\exp(\mathrm{i}kX^{\varepsilon}(t))\right\} = \exp(-D_\alpha |k|^\alpha t)$ with $0 < \alpha < 2$. This corresponds to the convergence of the discrete random walk X_n (3.10) to the symmetric α-stable Lévy process (Lévy flight).

If we rescale the compound Poisson process $X(t)$ as

$$X^{\varepsilon}(t) = \varepsilon^{\frac{1}{2}}X(t/\varepsilon) = \varepsilon^{\frac{1}{2}}\sum_{i=1}^{N(t/\varepsilon)} Z_i, \tag{3.203}$$

one can show that the random process $X^{\varepsilon}(t)$ converges to the Brownian motion $B(t)$ as well. This is the probabilistic explanation why the integral equation (3.74) can be approximated by the diffusion equation. However, if the second moment $\mathbb{E}(Z_i^2) = \infty$, then $X^{\varepsilon}(t)$ has other limiting processes, depending on the counting process $N(t)$.

3.6.2 Anomalous Scaling

So far we have discussed random walks with a finite mean waiting time and a finite variance of the jump length. These models lead to the classical parabolic scaling: $x \to x/\varepsilon^{1/2}$, $t \to t/\varepsilon$. The governing macroscopic equation for the density ρ becomes the standard diffusion equation. Let us now consider two cases for which the scaling is anomalous and the mean-field equations for ρ are fractional diffusion equations.

3.6.2.1 Finite Mean Waiting Time and Infinite Variance

Suppose that the jump PDF $w(z)$ is an even function and decreases as

$$w(z) \sim \frac{1}{|z|^{1+\alpha}}, \quad 0 < \alpha < 2, \tag{3.204}$$

for large z. It is clear that the second moment diverges for $0 < \alpha < 2$. The key question is how the rescaled process $X^{\varepsilon}(t) = \varepsilon^{H} X(t/\varepsilon)$ behaves as $\varepsilon \to 0$. Note that we rescale $X(t)$ by using a nontrivial scaling exponent H, the Hurst exponent. As before, we assume that the particle position $X(t)$ at time t is given by a CTRW

$$X(t) = \sum_{i=1}^{N(t)} Z_i, \tag{3.205}$$

where $N(t)$ is the Poisson process and the Z_i are random jumps with a heavy-tailed density (3.204). For simplicity, the jumps are assumed to be independent of the counting process $N(t)$. The waiting times between jumps are exponentially distributed with the mean value λ^{-1}. The generalized CLT ensures that

$$X^{\varepsilon}(t) = \varepsilon^{H} X(t/\varepsilon) = \varepsilon^{H} \sum_{i=1}^{N(t/\varepsilon)} Z_i \tag{3.206}$$

converges in distribution to a symmetric α-stable Lévy process, that is, $X^{\varepsilon}(t) \xrightarrow{\mathrm{d}} S_{\alpha}(t)$ as $\varepsilon \to 0$ [126] (see Sect. 3.3.3.2). The density of particles obeys the fractional diffusion equation

$$\frac{\partial \rho}{\partial t} = D_{\alpha} \frac{\partial^{\alpha} \rho}{\partial |x|^{\alpha}} \tag{3.207}$$

with $0 < \alpha < 2$. We conclude that stable Lévy processes are important for transport theory because they provide the macroscopic description of particles with heavy-tailed jumps in the hydrodynamic limit, $t \to \infty$ and $x \to \infty$.

From a probabilistic point of view, $S_{\alpha}(t)$ is the attractor for the rescaled particle position $X^{\varepsilon}(t)$. To understand this, consider first a discrete random walk. The rescaled position of a particle with jumps Z_i that are symmetric with respect to zero is $Y_n = n^{-1/\alpha} \sum_{i=1}^{n} Z_i$ with $0 < \alpha < 2$. We are interested in the limit $n \to \infty$, such that the sequence Y_n converges toward a "new" random variable Z in distribution, i.e., $Y_n \xrightarrow{\mathrm{d}} Z$ as $n \to \infty$ or $\lim_{n\to\infty} \mathbb{P}(Y_n < x) = \mathbb{P}(Z < x)$. The random variable Z is referred to as a symmetric *stable variable*. Since the parameter α plays a very important role, the random variable Z is said to be a symmetric α-stable random variable.

Recall that, in general, the stable random variable Z involves four parameters: the exponent (stable index) $0 < \alpha \leq 2$, the skewness $-1 \leq \beta \leq 1$, the shift $a \in \mathbb{R}$, and the scale $\sigma \geq 0$. It is well known that the stable probability density function

$$w(z|\alpha, \beta, \sigma, a) = \frac{\partial}{\partial z} \mathbb{P}(Z < z) \tag{3.208}$$

cannot be written in an explicit form, but its Fourier transform, the characteristic function has the following representation:

$$\tilde{w}(k|\alpha,\beta,\sigma,a) = \exp\left[\mathrm{i}ka - \sigma^{\alpha}\,|k|^{\alpha}\,(1 - \mathrm{i}\beta\,\mathrm{sgn}(k)\Omega)\right], \tag{3.209}$$

where $\Omega = \tan(\pi\alpha/2)$ for $\alpha \neq 1$ and $\Omega = -2/\pi \log|k|$ for $\alpha = 1$. The value $\beta = 0$ corresponds to a symmetric PDF. For example, the Cauchy distribution is

$$w(x|1,0,\sigma,a) = \frac{\sigma}{\pi\left[(x-a)^2 + \sigma^2\right]}, \tag{3.210}$$

for which $\alpha = 1$. We refer to Feller's book [126] for further details on stable random variables.

The generalized CLT states that if the jumps Z_i are symmetric around zero and distributed with heavy tails like $|z|^{-1-\alpha}$ for $z \to \infty$, then for a large number of steps n, the rescaled particle position $X_n/n^{1/\alpha}$ can be described by a symmetric α-stable distribution with $a = \beta = 0$. So if we choose $H = 1/\alpha$, then the rescaled particle position

$$X^{\varepsilon}(t) = \varepsilon^{H} \sum_{i=1}^{N(t/\varepsilon)} Z_i \tag{3.211}$$

tends to the symmetric α-stable Lévy process $S_{\alpha}(t)$ with the characteristic function $\mathbb{E}\left(\mathrm{e}^{\mathrm{i}kS_{\alpha}(t)}\right) = \mathrm{e}^{-D_{\alpha}|k|^{\alpha}t}$ and $D_{\alpha} = \lambda\sigma^{\alpha}$ (see (3.99)). The parameter D_{α} is referred to as a scale factor, which is a measure of the width of the density $\rho(x,t)$.

We conclude that as long as the mean waiting time and the variance of the jumps are finite, parabolic scaling leads to the Brownian motion in the limit $\varepsilon \to 0$. The *macroscopic* equation for the density of particles is a scale-invariant diffusion equation. Infinite variance of jumps in the domain of attraction of a stable law leads to Lévy processes, Lévy flights. In the limit $\varepsilon \to 0$, the particle position $X^{\varepsilon}(t)$ becomes self-similar with exponent $1/\alpha$. Recall that the random process $X(t)$ is *self-similar*, if there exists a scaling exponent H such that $X(t)$ and $\varepsilon^{H}X(t/\varepsilon)$ have the same distributions for any scaling parameter ε. In this case we write $X(t) \stackrel{\mathrm{d}}{=} \varepsilon^{H}X(t/\varepsilon)$. For a symmetric Lévy process with the characteristic function $\mathbb{E}\{\exp(\mathrm{i}kX(t))\} = \exp(-D_{\alpha}|k|^{\alpha}t)$, the scaling exponent is $H = 1/\alpha$. For the Brownian motion, $H = 1/2$. The main feature of a symmetric α-stable Lévy process is that it has independent heavy-tailed increments. The asymptotic behavior of the density of particles $\rho(x,t)$ for large x is

$$\rho(x,t) \sim \frac{D_{\alpha}t}{|x|^{1+\alpha}}. \tag{3.212}$$

In the three-dimensional case, the fractional diffusion equation in the long-time large-scale limit has the form

$$\frac{\partial \rho}{\partial t} = -D_\alpha (-\Delta)^{\frac{\alpha}{2}} \rho, \qquad \mathbf{x} \in \mathbb{R}^3, \tag{3.213}$$

in which the standard Laplacian Δ is replaced by a fractional Riesz operator. This replacement leads to a faster spread of particles, than the standard diffusion equation describes, i.e., superdiffusion, see Sect. 2.3. This is due to the heavy tails of the dispersal kernel $w(\mathbf{z}) \sim |\mathbf{z}|^{-d-\alpha}$ with $0 < \alpha < 2$ as $\mathbf{z} \to \infty$ where d is the dimension of space, $\mathbb{R}^d$. The underlying stochastic process is the rotationally invariant α-stable process [15]. A careful discussion of stable distributions and corresponding random processes is provided in [373, 444].

3.6.2.2 Infinite Mean Waiting Time and Infinite Variance of Jumps

Assume that the PDF of the waiting time $\phi(t)$ decreases like $t^{-1-\gamma}$ as $t \to \infty$, and particles have a dispersal kernel $w(z)$ with heavy tails $|z|^{-1-\alpha}$. What is the scale-invariant *macroscopic* equation for the particles density in this case? It turns out that the infinite variance of jumps leads to a fractional space derivative, and the infinite mean waiting time leads to the fractional Caputo derivative. The density of particles obeys the time–space fractional diffusion equation

$$\frac{\partial^\gamma \rho}{\partial t^\gamma} = D_{\alpha,\gamma} \frac{\partial^\alpha \rho}{\partial |x|^\alpha} \tag{3.214}$$

and the scale invariance relation

$$\rho(x,t) = \frac{1}{\varepsilon^{\frac{\gamma}{\alpha}}} \rho\left(\frac{x}{\varepsilon^{\frac{\gamma}{\alpha}}}, \frac{t}{\varepsilon}\right). \tag{3.215}$$

Note that the underlying stochastic process $S_{\alpha,\gamma}$ is not Markovian ($0 < \gamma < 1$) [371].

Let us show how the standard diffusion equation (3.16) and anomalous diffusion equation (3.214) emerge as a result of long-time large-scale limit of a CTRW described by (3.53). If we use the Dirac delta-function as the initial condition, then $\tilde{\rho}_0(k) = 1$, and the Fourier–Laplace transform of $\rho(x,t)$, (3.53), is given by

$$\hat{\tilde{\rho}}(k,s) = \frac{1 - \hat{\phi}(s)}{s\left[1 - \tilde{w}(k)\hat{\phi}(s)\right]}. \tag{3.216}$$

First we rescale $\hat{\tilde{\rho}}(k,s)$ as $\rho^\varepsilon(k,s) = \hat{\tilde{\rho}}\left(\varepsilon^H k, \varepsilon s\right)$ and use the standard expansions

$$\tilde{w}\left(\varepsilon^H k\right) = 1 - \frac{\sigma^2 \varepsilon^{2H} k^2}{2} + o\left(\varepsilon^{2H}\right), \tag{3.217}$$

$$\hat{\phi}(\varepsilon s) = 1 - \overline{T}\varepsilon s + o(\varepsilon). \tag{3.218}$$

If we choose scaling exponent $H = 1/2$, we obtain

$$\lim_{\varepsilon \to 0} \rho^{\varepsilon}(k, s) = \frac{1}{s + Dk^2}, \tag{3.219}$$

with $D = \sigma^2/2\overline{T}$. This corresponds to the standard diffusion equation; in the long-time large-scale limit all details of the random walk become irrelevant.

Consider now the anomalous case with the following scaling behavior:

$$\tilde{w}\left(\varepsilon^H k\right) = 1 - \frac{\sigma^{\alpha}\varepsilon^{H\alpha}\,|k|^{\alpha}}{2} + o\left(\varepsilon^{\alpha H}\right), \tag{3.220a}$$

$$\hat{\phi}(\varepsilon s) = 1 - \tau_0^{\gamma}(\varepsilon s)^{\gamma} + o\left(\varepsilon^{\gamma}\right). \tag{3.220b}$$

Substitution of these expressions into (3.216) yields the rescaled density $\rho^{\varepsilon}(k, s) = \hat{\hat{\rho}}\left(\varepsilon^H k, \varepsilon s\right)$. To obtain a nontrivial limit $\lim_{\varepsilon \to 0} \rho^{\varepsilon}(k, s)$, we have to choose

$$H = \frac{\gamma}{\alpha} \tag{3.221}$$

such that

$$\lim_{\varepsilon \to 0} \rho^{\varepsilon}(k, s) = \frac{s^{\gamma - 1}}{s^{\gamma} + D_{\alpha,\gamma} k^{\alpha}}, \tag{3.222}$$

which is the Fourier–Laplace transform of the fundamental solution of the time–space fractional equation (3.214) with

$$D_{\alpha,\gamma} = \frac{\sigma^{\alpha}}{2\tau_0^{\gamma}}. \tag{3.223}$$

Further details on the Cauchy problem for the time–space fractional diffusion equation (3.214) and its extension for the asymmetric case can be found in [371, 260].

Let us examine more closely the nature of the underlying stochastic process $S_{\alpha,\gamma}(t)$ for the time–space fractional equation (3.214). The latter is the long-time large-scale limit of the generalized Master equation (3.43) under the conditions that the symmetric jumps have a heavy-tailed density (3.204) with infinite variance and the waiting time PDF $\phi(t)$ decreases like $t^{-1-\gamma}$ with the index $0 < \gamma < 1$ as $t \to \infty$. Let us find the long-time large-scale limit of the CTRW under these conditions. We have introduced the CTRW as a subordinated stochastic process $X(t) = X_{N(t)}$ in which the parent process X_n is the position of a particle (3.10) in the discrete-time random walk (DTRW) model and the counting process $N(t)$ plays the role of the randomized time or operational time (see (3.26)). We have shown that

under the anomalous scaling $x \to x/\varepsilon^{1/\alpha}$, $t \to t/\varepsilon$, the discrete random walk X_n (3.10) converges to the symmetric α-stable Lévy process $S_\alpha(t)$, i.e.,

$$\varepsilon^{1/\alpha} X_{[t/\varepsilon]} \xrightarrow{\mathrm{d}} S_\alpha(t) \tag{3.224}$$

as $\varepsilon \to 0$. It can be shown that the rescaled counting process converges as

$$\varepsilon^{\gamma} N\left(\frac{t}{\varepsilon}\right) \xrightarrow{\mathrm{d}} N_\gamma(t) \tag{3.225}$$

If we compose these two processes, we obtain the subordinated process

$$S_{\alpha,\gamma}(t) = S_\alpha(N_\gamma(t)), \tag{3.226}$$

which is the scaling limit of the CTRW we are looking for. Note that $N_\gamma(t)$ is the hitting time: $N_\gamma(t) = \inf(\tau : T_\gamma(\tau) > t)$ for the γ-stable subordinator $T_\gamma(\tau)$. The latter is the scaling limit of the time of the nth jump T_n,

$$\varepsilon^{1/\gamma} T_{[t/\varepsilon]} = \varepsilon^{1/\gamma} \sum_{i=1}^{[t/\varepsilon]} \Theta_i \xrightarrow{\mathrm{d}} T_\gamma(t), \tag{3.227}$$

as $\varepsilon \to 0$. Here $\Theta_i = T_i - T_{i-1}$ is the interval between jumps. The non-Markovian behavior of the inverse subordinator $N_\gamma(t)$ leads to the non-Markovian behavior of $S_{\alpha,\gamma}(t)$. Of course, the scaling limit $S_{\alpha,\gamma}(t)$ is a self-similar process: $S_{\alpha,\gamma}(t) \overset{d}{=} \varepsilon^{\gamma/\alpha} S_{\alpha,\gamma}(t/\varepsilon)$. For further details and the statistical analysis of the relation between rescaled CTRWs and fractional equations, we refer to the series of papers by Meerschaert and his colleagues [39, 275, 277, 276, 278, 22, 25].

In Fig. 3.2 we present a schematic picture of the convergence from microscopic to macroscopic levels of description for different scalings and processes.

3.6.3 Scaling and Convergence to the Diffusion Process

We have seen how the scaling procedure can be used to obtain a *macroscopic* standard or fractional diffusion equation. We now describe the method for obtaining *macroscopic* equations without deriving *mesoscopic* balance equations like (3.13), (3.41), or (3.74). Let us explain the usefulness of the rescaling procedure. When *mesoscopic* balance equations are derived from some underlying *microscopic* random walk models, certain simplifying assumptions are made regarding the statistical characteristics of random movements. However, if the assumptions are less restrictive, we might have some problems deriving closed balance equations for the particle density. In fact, in many cases we will not be able to do so.

Consider the *microscopic* stochastic equation for the particle position $X(t)$,

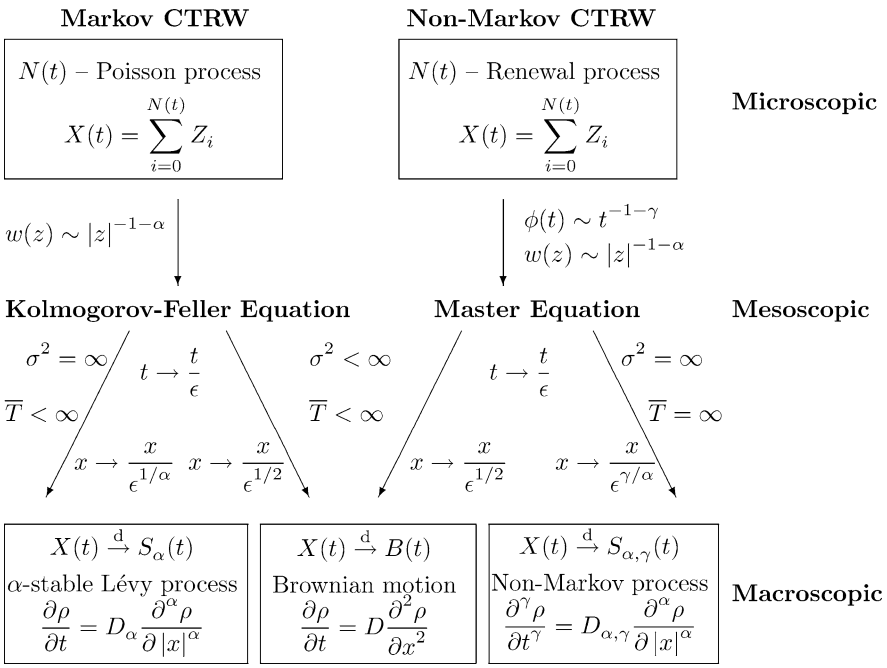

Fig. 3.2 Schematic picture for transition from microscopic to macroscopic equations

$$\frac{\mathrm{d}X}{\mathrm{d}t} = v\left(\varepsilon^{1/2}X(t), \xi(t)\right), \tag{3.228}$$

where the velocity v is a slowly varying function of the space coordinate x; $\varepsilon^{1/2}$ is a small parameter. We assume that v depends on some stationary random process $\xi(t)$ with zero mean. Under quite general conditions, the rescaled particle position, $X^{\varepsilon}(t) = \varepsilon^{\frac{1}{2}} X(t/\varepsilon)$, tends to a diffusion process as $\varepsilon \to 0$. The key question is how to find the effective velocity and diffusivity in the corresponding Fokker–Planck equation.

Before dealing with the general stochastic equation (3.228), it is useful for fixing the basic ideas to discuss a relatively simple example. Consider the equation for the particle position $X(t)$:

$$\frac{\mathrm{d}X}{\mathrm{d}t} = v(t), \tag{3.229}$$

where the random velocity $v(t)$ has zero mean and takes a finite number of values at random times T_n. We define the discrete Markov process (v_n, T_n), where v_n represents the velocity of the particle at the nth transition and T_n represents the random time at which the nth transition occurs. We assume that successive waiting times $T_n - T_{n-1}$ are independent identically distributed positive random variables. Even

under these assumptions, it is impossible to derive a closed equation for the PDF for the particle position or the mean density $\rho(x,t)$. To solve this problem, we need to make further simplifying assumptions regarding the velocity $v(t)$. Obviously, if $v(t)$ is Gaussian white noise, then $X(t)$ is the Brownian motion.

Let us apply the scaling idea and determine the behavior of the rescaled particle position $X^{\varepsilon}(t) = \varepsilon^{\frac{1}{2}} X(t/\varepsilon)$ in the long-time limit $\varepsilon \to 0$. It follows from (3.229) that $X^{\varepsilon}(t)$ with $X^{\varepsilon}(0) = 0$ can be written as

$$X^{\varepsilon}(t) = \varepsilon^{\frac{1}{2}} \int_0^{t/\varepsilon} v(s)\mathrm{d}s \approx \varepsilon^{\frac{1}{2}} \sum_{i=1}^{N(t/\varepsilon)} Y_i, \tag{3.230}$$

where $N(t) = \max\left\{n : T_n \le t\right\}$ is the random number of jumps in particle's velocity up to time t, $Y_i = v_{i-1}(T_i - T_{i-1})$ are IID random variables with zero mean and variance $\sigma_Y^2 = \mathbb{E}\{v_{i-1}^2 (T_i - T_{i-1})^2\}$, and $T_0 = 0$. Our goal is to show that $X^{\varepsilon}(t)$ converges in distribution to the Brownian motion $B(t)$ as $\varepsilon \to 0$. The important question is how the rescaled process $\varepsilon N(t/\varepsilon)$ behaves as $\varepsilon \to 0$. The renewal theorem states that if the mean waiting time between jumps $\overline{T} = \mathbb{E}\left\{T_i - T_{i-1}\right\}$ is finite, then $\varepsilon N(t/\varepsilon) \to t/\overline{T}$ as $\varepsilon \to 0$ [81]. The characteristic function $\mathbb{E}\left\{\exp\left(\mathrm{i}kX^{\varepsilon}(t)\right)\right\}$ can be written as $\mathbb{E}\left\{\exp\left(\mathrm{i}k\varepsilon^{\frac{1}{2}} \sum_{i=1}^{N(t/\varepsilon)} Y_i\right)\right\} \approx \left(\mathbb{E}\left\{\exp\left(\mathrm{i}k\varepsilon^{\frac{1}{2}} Y_i\right)\right\}\right)^{t/\varepsilon\overline{T}}$. Since $\mathbb{E}\left\{Y_i\right\} = 0$, we can write $\mathbb{E}\left\{\exp\left(\mathrm{i}kX^{\varepsilon}(t)\right)\right\} = \left(1 - k^2\varepsilon\sigma_Y^2/2 + o(\varepsilon)\right)^{t/\varepsilon\overline{T}} \to \exp\left(-Dk^2 t\right)$ as $\varepsilon \to 0$. So $X^{\varepsilon}(t)$ converges in distribution to $B(t)$ with the diffusion coefficient $D = \sigma_Y^2/2\overline{T}$.

For the general stochastic equation (3.228), the rescaled particle position $X^{\varepsilon}(t) = \varepsilon^{\frac{1}{2}} X(t/\varepsilon)$ tends to a diffusion process, in the limit $\varepsilon \to 0$, with the probability density function $p(x,t)$. The latter obeys the Fokker–Planck equation

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}(\mu(x)p) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left(\sigma^2(x)p\right), \tag{3.231}$$

with infinitesimal displacement

$$\mu(x) = \lim_{\varepsilon\to 0} \int_0^{1/\varepsilon} \int_0^{1/\varepsilon} \mathbb{E}_{\xi}\left[\frac{\partial v(x,\xi(s))}{\partial x} v(x,\xi(t))\right] \mathrm{d}s\mathrm{d}t \tag{3.232}$$

and infinitesimal variance $\sigma^2(x)$,

$$\sigma^2(x) = \lim_{\varepsilon\to 0} \int_0^{1/\varepsilon} \int_0^{1/\varepsilon} \mathbb{E}_{\xi}\left[v(x,\xi(s))v(x,\xi(t))\right] \mathrm{d}s\mathrm{d}t. \tag{3.233}$$

The details of the derivation can be found in [142].

3.7 Transport Equations and Underlying Stochastic Processes

In this section we remind the reader of the Kolmogorov forward and backward equations, infinitesimal generators, stochastic differential equations, and functional integrals and then consider how the basic transport equations are related to underlying Markov stochastic processes [141, 142].

3.7.1 Brownian Motion, Lévy Flight, and the Diffusion Equations

We start with a very simple one-dimensional diffusion equation

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2}, \quad x \in \mathbb{R}, \tag{3.234}$$

with the initial condition

$$\rho(x, 0) = \rho_0(x). \tag{3.235}$$

The solution of the initial value problem (3.234) and (3.235) can be written as

$$\rho(x, t) = \int_{\mathbb{R}} \rho_0(y)\, p(y, t|x)\mathrm{d}y, \tag{3.236}$$

where the Green's function, the propagator, is

$$p(y, t|x) = \frac{1}{\sqrt{4Dt}} \exp\left(-\frac{(y-x)^2}{4Dt}\right). \tag{3.237}$$

It should be noted that we integrate with respect to the "forward" variable y in (3.236). In this case, (3.236) has a very nice probabilistic interpretation. Consider the Brownian motion $B(t)$, which is a stochastic process with independent increments, such that $B(t + s) - B(s)$ is normally distributed with zero mean and variance $2Dt$. The corresponding transition probability density function $p(y, t|x)$ is given by (3.237). Therefore the solution (3.236) has a probabilistic representation

$$\rho(x, t) = \mathbb{E}_x \rho_0(B(t)), \tag{3.238}$$

where $\mathbb{E}_x$ is the expectation operator with respect to the random process $B(t)$ starting at point x. At first glance, (3.238) appears to provide the connection between the *microscopic* Brownian motion $B(t)$ and the *macroscopic* diffusion equation for the density of particles that all follow the Brownian motion. This is not quite true. Since we integrate with respect to the "forward" variable y, we treat (3.234) as the Kolmogorov backward equation which does not represent the transport equation. If

we integrate with respect to the "backward" variable x, then

$$\rho(y,t) = \int_{\mathbb{R}} \rho_0(x) p(y,t|x) \mathrm{d}x \tag{3.239}$$

is the solution to the Kolmogorov forward equation,

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial y^2}, \quad y \in \mathbb{R}, \tag{3.240}$$

with $\rho(y,0) = \rho_0(y)$.

Of course (3.234) and (3.240) are identical in form, but only the forward equation (3.240) has the physical meaning of a transport equation for particles. We will discuss the difference between forward and backward equations in the next section. It turns out that, it is more convenient to deal with the backward equation (3.234). Let us give an example. The Brownian motion $B(t)$ starting at x can be rewritten in terms of the standard Wiener process $W(t)$ as

$$B(t) = x + \sqrt{2D} W(t). \tag{3.241}$$

Recall that $W(0) = 0$, $\mathbb{E}W(t) = 0$, and $\mathbb{E}W^2(t) = t$. The solution to (3.234) and (3.235) can be written as

$$\rho(x,t) = \mathbb{E}\rho_0\Big(x + \sqrt{2D} W(t)\Big), \tag{3.242}$$

where $\mathbb{E}$ is the expectation operator with respect to $W(t)$. The main advantage of the probabilistic representation (3.242) is that we can use a Monte Carlo approach to estimate $\rho(x,t)$:

$$\rho(x,t) \approx \frac{1}{N} \sum_{i=1}^{N} \rho_0\Big(x + \sqrt{2Dt}\xi_i\Big), \tag{3.243}$$

where the sample ξ_i is computed from the standard normal distribution $\mathcal{N}(0,1)$ with zero mean and unit variance and N is the sample size [300]. The generalization of these ideas to a Brownian particle moving in three dimensions is straightforward. The solution of the Cauchy problem

$$\frac{\partial u}{\partial t} = D\Delta u, \quad u(\mathbf{x},0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3, \tag{3.244}$$

can be written as

$$u(\mathbf{x},t) = \mathbb{E}u_0\Big(\mathbf{x} + \sqrt{2D}\mathbf{W}(t)\Big), \tag{3.245}$$

where $\mathbf{W}(t)$ is the standard three-dimensional Wiener process.

The probabilistic solution to the space-fractional Cauchy problem

$$\frac{\partial u}{\partial t} = D_\alpha \frac{\partial^\alpha u}{\partial |x|^\alpha}, \quad u(x,0) = u_0(x), \quad x \in \mathbb{R}, \tag{3.246}$$

can be written in terms of the symmetric α-stable Lévy motion $S_\alpha(t)$ (Lévy flight) as

$$u(x,t) = \mathbb{E} u_0\big(x + S_\alpha(t)\big), \tag{3.247}$$

where $S_\alpha(t)$ is defined in Sect. 3.3.3.2. Of course, for the simple transport problem (3.234) and (3.235) we have an explicit solution (3.236). In most cases, explicit solutions to the transport equations are not available, but we still can write down the solution in the form of the functional integral (3.238). In fact, this formula can be easily coded to obtain numerical solutions; it provides a powerful alternative to standard finite difference methods [300].

3.7.2 Transport Equations: Forward vs Backward

Consider a collection of particles that move independently of each other in three-dimensional space $\mathbb{R}^3$. We assume that the position of a particle $\mathbf{X}(t)$ is a time-homogeneous Markov process with transition density $p(\mathbf{y}, t|\mathbf{x})$.

The density of particles $\rho(\mathbf{y}, t)$ at point $\mathbf{y}$ at time t can be expressed in terms of the initial density of particles $\rho_0(\mathbf{x})$ as

$$\rho(\mathbf{y}, t) = \int_{\mathbb{R}^3} \rho_0(\mathbf{x}) p(\mathbf{y}, t|\mathbf{x}) \mathrm{d}\mathbf{x}, \tag{3.248}$$

where the integration is performed with respect to the "initial" or "backward" variable $\mathbf{x}$. This equation has a very simple meaning as the balance of particles arriving at point $\mathbf{y}$ from various initial positions $\mathbf{x}$. The probabilistic meaning of this equation is the law of total probability: the probability density $\rho(\mathbf{y}, t)$ is the sum (integral) of the probability density $p(\mathbf{y}, t|\mathbf{x})$ to be at point $\mathbf{y}$ at time t conditional on being at point $\mathbf{x}$ at $t = 0$ multiplied by the probability density $\rho_0(\mathbf{x})$ to be at point $\mathbf{x}$ at time 0.

We define a transport operator Q_t as follows:

$$\rho(\mathbf{y}, t) = Q_t \rho_0(\mathbf{y}) \equiv \int_{\mathbb{R}^3} \rho_0(\mathbf{x}) p(\mathbf{y}, t|\mathbf{x}) \mathrm{d}\mathbf{x}, \tag{3.249}$$

so the density of particles $\rho(\mathbf{y}, t)$ is the solution of a transport equation written in terms of the "forward" variable $\mathbf{y}$. The key question is what equation does $\rho(\mathbf{y}, t) = Q_t \rho_0(\mathbf{y})$ satisfy. In what follows, we derive several transport equations

corresponding to various random processes $\mathbf{X}(t)$ and probability density functions $p(\mathbf{y}, t|\mathbf{x})$, Green's functions.

As we have mentioned in the previous section, it is convenient to integrate with respect to the "forward" variable $\mathbf{y}$. We define the transition operator T_t and the new function $u(\mathbf{x}, t)$ as

$$u(\mathbf{x}, t) = T_t u_0(\mathbf{x}) \equiv \int_{\mathbb{R}^3} u_0(\mathbf{y}) p(\mathbf{y}, t|\mathbf{x}) \mathrm{d}\mathbf{y}, \tag{3.250}$$

where $u(\mathbf{x}, 0) = u_0(\mathbf{x})$. We use the notation u instead of ρ to emphasize that the function $u(\mathbf{x}, t)$ is formal and does not generally represent the particle density.

It follows from (3.250) that the operator T_t, associated with the transition probability $p(\mathbf{y}, t|\mathbf{x})$, can be written in terms of a conditional expectation $\mathbb{E}_{\mathbf{x}}$ over the particle position $\mathbf{X}(t)$ at time t, provided $\mathbf{X}(0) = \mathbf{x}$:

$$T_t f(\mathbf{x}) = \mathbb{E}_{\mathbf{x}} f(\mathbf{X}(t)). \tag{3.251}$$

We always write the expectation $\mathbb{E}_{\mathbf{x}}$ with the index $\mathbf{x}$ when we want to emphasize that the process $\mathbf{X}(t)$ starts at point $\mathbf{x}$, i.e., $\mathbf{X}(0) = \mathbf{x}$:

$$\mathbb{E}_{\mathbf{x}} \{f(\mathbf{X}(t))\} = \mathbb{E} \{f(\mathbf{X}(t))|\mathbf{X}(0) = \mathbf{x}\}. \tag{3.252}$$

The operator T_t has the semigroup property, $T_t T_s f = T_{t+s} f$. It is easy to check that T_t is the adjoint of Q_t:

$$\int_{\mathbb{R}^3} T_t f(\mathbf{x}) \varphi(\mathbf{x}) \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} f(\mathbf{x}) Q_t \varphi(\mathbf{x}) \mathrm{d}\mathbf{x}. \tag{3.253}$$

We conclude that if the operator T_t is self-adjoint, i.e., $T_t = Q_t$, then it can be used as a transport operator. If the random position $\mathbf{X}(t)$ of a particle starting at $\mathbf{x} = 0$ is a symmetric process for which $\mathbb{P}(\mathbf{X}(t) = \mathbf{x}) = \mathbb{P}(\mathbf{X}(t) = -\mathbf{x})$, then the operator T_t is self-adjoint. For example, the Brownian motion $B(t)$ is a symmetric process. Note that if a stationary distribution $\overline{\rho}(\mathbf{y})$ exists, it satisfies $\overline{\rho}(\mathbf{y}) = Q_t \overline{\rho}(\mathbf{y})$.

Let us define two evolution operators L and L^* for the Markov process $\mathbf{X}(t)$:

$$Lf(\mathbf{x}) = \lim_{h \to 0} \frac{T_h f(\mathbf{x}) - f(\mathbf{x})}{h} = \lim_{h \to 0} \frac{\int_{\mathbb{R}^3} f(\mathbf{y}) p(\mathbf{y}, h|\mathbf{x}) \mathrm{d}\mathbf{y} - f(\mathbf{x})}{h}, \tag{3.254}$$

where L acts only on the "backward" variable $\mathbf{x}$, and

$$L^* f(\mathbf{y}) = \lim_{h \to 0} \frac{Q_h f(\mathbf{y}) - f(\mathbf{y})}{h} = \lim_{h \to 0} \frac{\int_{\mathbb{R}^3} f(\mathbf{x}) p(\mathbf{y}, h|\mathbf{x}) \mathrm{d}\mathbf{x} - f(\mathbf{y})}{h}, \tag{3.255}$$

where L^* acts on the "forward" variable $\mathbf{y}$. The operators L and L^* are called the infinitesimal generators of the semigroups T_t and Q_t, respectively [142]. The operator L^* is the adjoint of L:

$$\int_{\mathbb{R}^3} L^* f(\mathbf{x})\varphi(\mathbf{x})\mathrm{d}\mathbf{x} = \int_{\mathbb{R}^3} f(\mathbf{x}) L\varphi(\mathbf{x})\mathrm{d}\mathbf{x}. \tag{3.256}$$

One can show that $u(\mathbf{x}, t)$ given by (3.250) is the unique solution of the initial-value problem:

$$\frac{\partial u}{\partial t} = Lu, \quad u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3. \tag{3.257}$$

The function $\rho(\mathbf{y}, t)$ given by (3.248) obeys the following initial-value problem:

$$\frac{\partial \rho}{\partial t} = L^* \rho, \quad \rho(\mathbf{y}, 0) = \rho_0(\mathbf{y}), \quad \mathbf{y} \in \mathbb{R}^3. \tag{3.258}$$

Note that some authors have used these operators interchangeably for the description of the mesoscopic transport process. It is clear that if L is self-adjoint, then it can be used as a transport operator and the function $u(\mathbf{x}, t)$ can represent the particle density. For example, the one-dimensional Brownian motion $B(t)$ has the infinitesimal generator $L = \partial^2/\partial x^2$ which is self-adjoint. A symmetric α-stable Lévy process on $\mathbb{R}$ has the generator $L = \partial^\alpha/\partial\,|x|^\alpha$, which is self-adjoint too. In the next section we obtain L and L^* from the Chapman–Kolmogorov equation.

3.7.3 Chapman–Kolmogorov Equation and Infinitesimal Generators

Let us consider the Chapman–Kolmogorov equation for the transition density $p(\mathbf{y}, t|\mathbf{x})$:

$$p(\mathbf{y}, t + s|\mathbf{x}) = \int_{\mathbb{R}^3} p(\mathbf{z}, t|\mathbf{x}) p(\mathbf{y}, s|\mathbf{z})\mathrm{d}\mathbf{z}. \tag{3.259}$$

Our goal is to derive the Kolmogorov forward and backward equations and to discuss the main difference between them. The forward equation deals with the events during the small time interval $(t, t+h]$ and gives us the answer for how those events define the probability density $p(\mathbf{y}, t+h|\mathbf{x})$ at time $t+h$, while the backward equation is concerned with events just after the time $t = 0$.

Let us replace s with small h in (3.259) and rewrite this equation for the density $\rho(\mathbf{y}, t)$:

$$\rho(\mathbf{y}, t + h) = \int_{\mathbb{R}^3} \rho(\mathbf{z}, t) p(\mathbf{y}, h|\mathbf{z})\mathrm{d}\mathbf{z}, \tag{3.260}$$

where $p(\mathbf{y}, h|\mathbf{z})$ represents the probability of the transitions from $\mathbf{z}$ to $\mathbf{y}$ occurring during short time interval $(t, t + h]$. The meaning of this equation is very simple. It gives the balance of particles at point $\mathbf{y}$ at time $t + h$. Subtracting $\rho(\mathbf{y}, t)$ from both sides and dividing by h, we find

$$\frac{\rho(\mathbf{y}, t+h) - \rho(\mathbf{y}, t)}{h} = \frac{\int_{\mathbb{R}^3} \rho(\mathbf{z}, t) p(\mathbf{y}, h|\mathbf{z}) \mathrm{d}\mathbf{z} - \rho(\mathbf{y}, t)}{h}. \tag{3.261}$$

Letting $h \to 0$, we obtain the Kolmogorov forward equation, the Master equation,

$$\frac{\partial \rho(\mathbf{y}, t)}{\partial t} = L^* \rho(\mathbf{y}, t), \tag{3.262}$$

where L^* is defined by (3.255). The transition probability $p(\mathbf{y}, t|\mathbf{x})$ obeys the same equation with respect to the forward variable $\mathbf{y}$. The main idea in the derivation of (3.262) is to split the time interval $(0, t+h]$ into a long interval $(0, t]$ and a short interval $(t, t+h]$, so that the particle density at time $t+h$ is the result of transitions during the short time interval $(t, t+h]$.

To derive the backward equation, we consider the events just after the time $t = 0$ during the short time interval $(0, h]$. The Chapman–Kolmogorov equation is

$$p(\mathbf{y}, h+t|\mathbf{x}) = \int_{\mathbb{R}^3} p(\mathbf{z}, h|\mathbf{x}) p(\mathbf{y}, t|\mathbf{z}) \mathrm{d}\mathbf{z}. \tag{3.263}$$

We cannot write a similar equation for the density $\rho(\mathbf{x}, h+t)$. Rewriting (3.263) as

$$\frac{p(\mathbf{y}, h+t|\mathbf{x}) - p(\mathbf{y}, t|\mathbf{x})}{h} = \frac{\int_{\mathbb{R}^3} p(\mathbf{z}, h|\mathbf{x}) p(\mathbf{y}, t|\mathbf{z}) \mathrm{d}\mathbf{z} - p(\mathbf{y}, t|\mathbf{x})}{h}, \tag{3.264}$$

we obtain, in the limit $h \to 0$, the Kolmogorov backward equation

$$\frac{\partial p(\mathbf{y}, t|\mathbf{x})}{\partial t} = L p(\mathbf{y}, t|\mathbf{x}). \tag{3.265}$$

This equation is written for two variables, the time t and the initial position $\mathbf{x}$. The final position $\mathbf{y}$ plays the role of a parameter. The function $u(x, t)$ defined in (3.250) obeys the Kolmogorov backward equation:

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} = L u(\mathbf{x}, t). \tag{3.266}$$

The natural question arises whether this equation represents the mesoscopic transport of particles. The answer in general is negative. In what follows we illustrate a general technique, using several examples of Markov processes.

3.7.3.1 Poisson Process

As a first illustration, consider the Poisson process $N_a(t)$ with intensity λ and jump size a. We assume that the process starts at the point x. Then

$$Lf(x) = \lim_{h \to 0} \frac{\mathbb{E}_x f(N_a(h)) - f(x)}{h} = \lambda(f(x+a) - f(x)). \tag{3.267}$$

Referring to (3.250) and (3.257), we conclude that the solution to the finite difference backward equation

$$\frac{\partial u}{\partial t} = Lu = \lambda(u(x+a,t) - u(x,t)), \quad x \in \mathbb{R}, \tag{3.268}$$

with the initial condition $u(x,0) = u_0(x)$, can be written as

$$u(x,t) = T_t u_0(x) = \mathbb{E}_x u_0(N_a(t)) = \sum_{k=0}^{\infty} u_0(x+ak) \frac{\mathrm{e}^{-\lambda t}(\lambda t)^k}{k!}. \tag{3.269}$$

As usual we use the notation $\mathbb{E}_x$ to emphasize that the expectation is taken with respect to the process $N_a(t)$ starting at x.

The forward equation follows from the balance equation (3.74) with $w(z) = \delta(z-a)$, i.e.,

$$\frac{\partial \rho}{\partial t} = L^* \rho = \lambda(\rho(y-a,t) - \rho(y,t)), \quad y \in \mathbb{R}. \tag{3.270}$$

The advantage of having a probabilistic solution (3.269) is that it helps us to find an explicit solution of the Cauchy problem for the transport equation (3.270) by changing the sign $a \to -a$:

$$\rho(y,t) = Q_t \rho_0(y) = \sum_{k=0}^{\infty} \rho_0(y-ak) \frac{\mathrm{e}^{-\lambda t}(\lambda t)^k}{k!}. \tag{3.271}$$

3.7.3.2 Three-Dimensional Brownian motion

As another illustration, consider the Brownian motion $\mathbf{B}(t)$ in three dimensions starting at point $\mathbf{x}$. The operator L is the Laplacian, i.e.,

$$Lf(\mathbf{x}) = \lim_{h \to 0} \frac{\mathbb{E}_{\mathbf{x}} f(\mathbf{B}(h)) - f(\mathbf{x})}{h} = D\Delta f. \tag{3.272}$$

The solution of the Kolmogorov backward diffusion equation

$$\frac{\partial u(\mathbf{x},t)}{\partial t} = D\Delta u(\mathbf{x},t), \quad \mathbf{x} \in \mathbb{R}^3, \tag{3.273}$$

with the initial condition $u(\mathbf{x},0) = u_0(\mathbf{x})$, can be written as

$$u(\mathbf{x},t) = T_t u_0(\mathbf{x}) = \mathbb{E}_{\mathbf{x}} u_0(\mathbf{B}(t)) = \int_{\mathbb{R}^3} \rho_0(\mathbf{x}+\mathbf{z}) \frac{\mathrm{e}^{-\mathbf{z}\cdot\mathbf{z}/(4Dt)}}{(4\pi Dt)^{3/2}} \mathrm{d}\mathbf{z}. \tag{3.274}$$

The operator L is self-adjoint, and the transport equation for the density is of the form

$$\frac{\partial \rho(\mathbf{y}, t)}{\partial t} = D\Delta\rho(\mathbf{y}, t), \quad \mathbf{y} \in \mathbb{R}^3. \tag{3.275}$$

The solution to this equation with the initial condition $\rho(\mathbf{y}, 0) = \rho_0(\mathbf{y})$ is $\rho(\mathbf{y}, t) = \mathbb{E}_{\boldsymbol{y}}\rho_0(\mathbf{B}(t))$. In this case $\mathbf{B}(t)$ starts at point $\boldsymbol{y}$.

3.7.3.3 Deterministic Motion

Consider the case where the particles move with deterministic velocity $\mathbf{v}(\mathbf{x})$:

$$\frac{\mathrm{d}\mathbf{X}(t)}{\mathrm{d}t} = \mathbf{v}(\mathbf{X}(t)), \quad \mathbf{X}(0) = \mathbf{x}, \quad \mathbf{x} \in \mathbb{R}^3. \tag{3.276}$$

Then

$$Lf(\mathbf{x}) = \lim_{h\to 0} \frac{f(\mathbf{X}(h)) - f(\mathbf{x})}{h} = \mathbf{v}(\mathbf{x}) \cdot \nabla f = \sum_i v_i(\mathbf{x}) \frac{\partial f}{\partial x_i}. \tag{3.277}$$

The initial value problem

$$\frac{\partial u}{\partial t} = Lu = \mathbf{v}(\mathbf{x}) \cdot \nabla u, \quad u(\mathbf{x}, 0) = u_0(\mathbf{x}) \tag{3.278}$$

has the solution

$$u(\mathbf{x}, t) = T_t u_0(\mathbf{x}) = u_0(\mathbf{X}(t)). \tag{3.279}$$

The backward equation, Liouville's equation, for the particle density takes the form

$$\frac{\partial \rho}{\partial t} = L^*\rho = -\sum_i \frac{\partial}{\partial y_i}(v_i(\mathbf{y})\rho). \tag{3.280}$$

For incompressible flow where $\nabla \cdot \mathbf{v} = 0$ we obtain the transport equation

$$\frac{\partial \rho}{\partial t} + \mathbf{v}(\mathbf{y}) \cdot \nabla\rho = 0. \tag{3.281}$$

This equation, together with the initial condition $\rho(\mathbf{y}, 0) = \rho_0(\mathbf{y})$, is identical to (3.278) if we change the direction of velocity field $\mathbf{v} \to -\mathbf{v}$. That is why we can write

$$\rho(\mathbf{y}, t) = \rho_0(\mathbf{X}(t)), \tag{3.282}$$

where $\mathbf{X}(t)$ is the solution of the initial value problem

$$\frac{\mathrm{d}\mathbf{X}(t)}{\mathrm{d}t} = -\mathbf{v}(\mathbf{X}(t)), \quad \mathbf{X}(0) = \mathbf{y}. \tag{3.283}$$

Later we will see how the deterministic theory above can be extended to the convection–diffusion equation of the form

$$\frac{\partial \rho}{\partial t} + \mathbf{v}(\mathbf{y}) \cdot \nabla \rho = D\Delta\rho. \tag{3.284}$$

3.7.3.4 Discrete-in-Space Random Walk

Let $X(t)$ be the position of a particle performing a random walk on the x-axis. If the particle is at point x at time t, then the probability that it will jump to the right, to the point $x + a$, during $(t, t + h]$ is $\alpha(x)h + o(h)$. The probability of a jump to the left to $x - a$ at time $t + h$ is $\beta(x)h + o(h)$. The probability of no jumps is $1 - \alpha(x)h - \beta(x)h + o(h)$. These transition probabilities allow us to find the infinitesimal operator L:

$$Lf(x) = \lim_{h\to 0} \frac{\mathbb{E}_x f(X(h)) - f(x)}{h} = \alpha(x)(f(x + a) - f(x)) + \beta(x)(f(x - a) - f(x)). \tag{3.285}$$

So the Kolmogorov backward equation is

$$\frac{\partial u}{\partial t} = Lu = \alpha(x)\left[u(x + a, t) - u(x)\right] + \beta(x)\left[u(x - a, t) - u(x, t)\right]. \tag{3.286}$$

For the initial condition $u(x, 0) = u_0(x)$, it has the solution $u(x, t) = \mathbb{E}_x u_0(X(t))$. The forward equation for the density of particles takes the form

$$\frac{\partial \rho}{\partial t} = L^*\rho = \alpha(y - a)\rho(y - a, t) - \alpha(y)\rho(y) + \beta(y + a)\rho(y + a, t) - \beta(y)\rho(y, t). \tag{3.287}$$

If the transition rates $\alpha = \beta = \text{const}$, then the forward and backward equations are identical. In particular, the mesoscopic equation for the density ρ is

$$\frac{\partial \rho}{\partial t} = \alpha(\rho(x + a, t) - 2\rho(x, t) + \rho(x - a, t)). \tag{3.288}$$

We see that (3.288) is simply a discrete-in-space version of the diffusion equation (3.234). On the right-hand side we have a symmetric central-difference approximation for the second derivative $D\partial^2\rho/\partial x^2$ with the diffusion coefficient $D = \alpha a^2$.

This suggests that if we let the step size $a \to 0$ and the rate $\alpha \to \infty$ such that $D = \alpha a^2$=const, the density $\rho(x,t)$ converges to the function that obeys the diffusion equation. The function $\rho(x,t) = \mathbb{E}_x \rho_0(X(t))$ represents a solution of the difference equation (3.288) with $\rho(x,0) = \rho_0(x)$ as an expectation with respect to the position of the random walk $X(t)$.

3.7.3.5 Markov Process with Jumps

Consider a particle that moves with a velocity $v(x)$ on $\mathbb{R}$ and jumps at random times so that the rate of jumps depends on the position of the particle. The one-dimensional microscopic movement can be represented as follows. If the position of the particle at time t is $X(t)$, then at time $t+h$ the position is

$$X(t+h) = X(t) + v(X(t))h + Z(t) + o(h), \tag{3.289}$$

with probability $\lambda(X(t))h + o(h)$, and

$$X(t+h) = X(t) + v(X(t))h + o(h) \tag{3.290}$$

with probability $1 - \lambda(X(t))h + o(h)$. The stationary random process $Z(t)$ has the conditional jump density

$$w(z|x) = \frac{\partial}{\partial z}\mathbb{P}\left\{Z(t) \le z | X(t) = x\right\}. \tag{3.291}$$

The Kolmogorov backward equation is

$$\frac{\partial u(x,t)}{\partial t} = Lu(x,t) = v(x)\frac{\partial u}{\partial x} + \lambda(x)\int_{\mathbb{R}} u(x+z,t)w(z|x)\mathrm{d}z - \lambda(x)u(x,t). \tag{3.292}$$

The Kolmogorov forward equation, the Master equation, for the density $\rho(y,t)$ is

$$\frac{\partial \rho(y,t)}{\partial t} = L^*\rho(y,t) = -\frac{\partial (v(y)\rho)}{\partial y} + \int_{\mathbb{R}} \lambda(y-z)\rho(y-z,t)w(z|y-z)\mathrm{d}z - \lambda(y)\rho(y,t). \tag{3.293}$$

If $\lambda = \text{const}$, $w(z)$ does not depend on x, and $v(x) = 0$, we obtain the Kolmogorov–Feller equation (3.74), for which the underlying microscopic random movement is a compound Poisson process.

3.7.3.6 Integral-Difference Equation and Discrete Random Walk

Consider the discrete-time random walk model for the particle position X_n,

$$X_{n+1} = X_n + Z_{n+1}, \tag{3.294}$$

where the sequence of independent random jumps Z_n is defined by the conditional density

$$w(z|x) = \frac{\partial}{\partial z}\mathbb{P}(Z_n \leq z|X_{n-1} = x). \tag{3.295}$$

The transition probability density function

$$p(y, n|x) = \frac{\partial}{\partial y}\mathbb{P}(X_n \leq y|X_0 = x) \tag{3.296}$$

obeys two equations [126]. The Kolmogorov forward equation involves the last jump that takes place at time $n - 1$:

$$p(y, n|x) = \int_{\mathbb{R}} p(y - z, n - 1|x)w(z|y - z)\mathrm{d}z \tag{3.297}$$

with $n = 1, 2, 3, \ldots$. The Kolmogorov backward equation deals with the first jump at time 1:

$$p(y, n|x) = \int_{\mathbb{R}} w(z|x)p(y, n - 1|x + z)\mathrm{d}z. \tag{3.298}$$

The Master equation for the density is

$$\rho(y, n) = \int_{\mathbb{R}} \rho(y - z, n - 1)w(z|y - z)\mathrm{d}z. \tag{3.299}$$

The backward equation for the function u takes the form

$$u(x, n) = \int_{\mathbb{R}} w(z|x)u(z, n - 1)\mathrm{d}z. \tag{3.300}$$

For even jump PDFs, i.e., $w(x) = w(-x)$, the backward and forward equations are identical in form.

3.7.3.7 One-Dimensional Diffusion Process

We have seen that an appropriate rescaling of time and renormalizing the stochastic process leads to the Brownian motion. Here we define the homogeneous-in-time

diffusion process $X(t)$, which has two basic statistical characteristics, the infinitesimal displacement (or drift) $\mu(x)$ and the infinitesimal variance $\sigma^2(x)$:

$$\mu(x) = \lim_{h\to 0} \frac{1}{h}\mathbb{E}\left\{X(t+h) - X(t)|X(t) = x\right\}, \tag{3.301}$$

$$\sigma^2(x) = \lim_{h\to 0} \frac{1}{h}\mathbb{E}\left\{\left[X(t+h) - X(t)\right]^2 |X(t) = x\right\}. \tag{3.302}$$

The diffusion process $X(t)$ can also be defined by the Itô stochastic differential equation (SDE)

$$\mathrm{d}X = \mu(X)\mathrm{d}t + \sigma(X)\mathrm{d}W, \tag{3.303}$$

where $W(t)$ is the standard Wiener process [141, 142]. It is clear that $W(t)$ can be defined as a diffusion process with $\mu(x) = 0$ and $\sigma^2(x) = 1$.

The conditional probability density function

$$p(y, t|x) = \frac{\partial}{\partial y}\mathbb{P}\left\{X(t) \le y|X(0) = x\right\} \tag{3.304}$$

satisfies the forward equation, the Fokker–Planck equation,

$$\frac{\partial p}{\partial t} = L^* p = -\frac{\partial}{\partial y}(\mu(y)p) + \frac{1}{2}\frac{\partial^2}{\partial y^2}\left(\sigma^2(y)p\right) \tag{3.305}$$

and the backward equation

$$\frac{\partial p}{\partial t} = Lp = \mu(x)\frac{\partial p}{\partial x} + \frac{\sigma^2(x)}{2}\frac{\partial^2 p}{\partial x^2}. \tag{3.306}$$

So the initial value problem

$$\frac{\partial u}{\partial t} = Lu, \quad u(x, 0) = u_0(x), \tag{3.307}$$

has the solution

$$u(x, t) = \mathbb{E}_x u_0(X(t)). \tag{3.308}$$

As we discussed earlier, the backward equation (3.307) does not describe the average transport process of particles that follow the process $X(t)$. The transport equation for the density $\rho(y, t)$ with the convection–diffusion flux $J = v(y)\rho - D(y)\partial\rho/\partial y$ can be written as

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial y}(v(y)\rho) + \frac{\partial}{\partial y}\left(D(y)\frac{\partial \rho}{\partial y}\right). \tag{3.309}$$

The convection–diffusion equation (3.309) has the form of a forward equation, $\partial\rho/\partial t = L^*\rho$, if

$$D(y) = \frac{\sigma^2(y)}{2}, \quad v(y) = \mu(y) - \sigma(y)\frac{\partial \sigma(y)}{\partial y}. \tag{3.310}$$

3.7.3.8 Diffusion Process in Three Dimensions

We discuss the diffusion process in three dimensions in the context of an anisotropic convection–diffusion equation for the density of particles. Our goal is to obtain the probabilistic solution to the initial value problem

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3} v_i(\mathbf{x})\frac{\partial \rho}{\partial x_i} = \sum_{i,j=1}^{3} \frac{\partial}{\partial x_i}\left(D_{ij}(\mathbf{x})\frac{\partial \rho}{\partial x_j}\right), \quad \rho(\mathbf{x}, 0) = \rho_0(\mathbf{x}). \tag{3.311}$$

Let us assume that the particle position $\mathbf{X}(t)$ is the solution to the Itô SDE

$$\mathrm{d}\mathbf{X}(s) = b(\mathbf{X}(s))\mathrm{d}s + \sigma(\mathbf{X}(s))\mathrm{d}\mathbf{W}(s), \quad \mathbf{X}(0) = \mathbf{x}, \quad 0 \le s \le t, \tag{3.312}$$

where $\mathbf{W}(s)$ is the standard three-dimensional Wiener process, and σ is the matrix of infinitesimal variances [141]. Using coordinate notation, we rewrite the SDE (3.312) in the integral form as

$$X_i(t) = x_i + \int_0^t b_i(\mathbf{X}(s))\mathrm{d}s + \int_0^t \sum_{j=1}^{3} \sigma_{ij}(\mathbf{X}(s))\mathrm{d}W_j(s), \quad i = 1, 2, 3. \tag{3.313}$$

This formula allows us to find the generator

$$\begin{aligned} Lf(\mathbf{x}) &= \lim_{h\to 0} \frac{\mathbb{E}_{\mathbf{x}} f(\mathbf{X}(h)) - f(\mathbf{x})}{h} \\ &= \sum_{i=1}^{3} b_i(\mathbf{x})\frac{\partial f(\mathbf{x})}{\partial x_i} + \sum_{i,j=1}^{3} D_{ij}(\mathbf{x})\frac{\partial f(\mathbf{x})}{\partial x_i \partial x_j}, \end{aligned} \tag{3.314}$$

where the diffusion matrix $\mathsf{D}(\mathbf{x})$ is given by

$$D_{ij}(\mathbf{x}) = \frac{1}{2}\sum_{k=1}^{3} \sigma_{ik}(\mathbf{x})\sigma_{kj}(\mathbf{x}). \tag{3.315}$$

The anisotropic convection–diffusion equation (3.311) can be written in the form of a backward equation, $\partial\rho/\partial t = L\rho$, if

$$b_i(\mathbf{x}) = -v_i(\mathbf{x}) + \sum_{k=1}^{3} \frac{\partial D_{ki}(\mathbf{x})}{\partial x_k}. \tag{3.316}$$

We know that the Cauchy problem

$$\frac{\partial u}{\partial t} = Lu, \quad u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3, \tag{3.317}$$

has the solution $u(\mathbf{x}, t) = \mathbb{E}_{\mathbf{x}} u_0(\mathbf{X}(t))$. Thus we conclude that the probabilistic solution to the initial value problem (3.311) is

$$\rho(\mathbf{x}, t) = \mathbb{E}_{\mathbf{x}} \rho_0(\mathbf{X}(t)), \tag{3.318}$$

where the random process $\mathbf{X}(t)$ is defined by the SDE (3.312) with (3.315) and (3.316).

It is instructive to show how the Itô formula can be used to obtain the probabilistic solution to (3.317) [141]. We consider a "new" Markov process $(\mathbf{X}(s), T(s))$, where the first component $\mathbf{X}(s)$ obeys (3.312) and the effective time $T(s)$ is defined as

$$T(s) = t - s, \quad 0 \le s \le t. \tag{3.319}$$

We apply the Itô formula to the smooth function $u(\mathbf{x}, t)$:

$$\begin{aligned} \mathrm{d}u(\mathbf{X}(s), T(s)) = \left[-\frac{\partial u}{\partial t}(\mathbf{X}(s), T(s)) + Lu(\mathbf{X}(s), T(s)) \right] \mathrm{d}s \\ + \nabla_{\mathbf{x}} u(\mathbf{X}(s), T(s)) \cdot \sigma(\mathbf{X}(s)) \mathrm{d}\mathbf{W}(s). \end{aligned} \tag{3.320}$$

This equation can be rewritten in the integral form as

$$\begin{aligned} u(\mathbf{X}(t), 0) - u(\mathbf{x}, t) = \int_0^t \left[-\frac{\partial u}{\partial t}(\mathbf{X}(s), t - s) + Lu(\mathbf{X}(s), t - s) \right] \mathrm{d}s \\ + \int_0^t \nabla_{\mathbf{x}} u(\mathbf{X}(s), t - s) \cdot \sigma(\mathbf{X}(s)) \mathrm{d}\mathbf{W}(s). \end{aligned} \tag{3.321}$$

If we average both sides and take into account (3.317), we obtain

$$u(\mathbf{x}, t) = \mathbb{E}_{\mathbf{x}} u_0(\mathbf{X}(t)). \tag{3.322}$$

3.7.4 Convection–Diffusion Equation with Reactions

This section is devoted to probabilistic solutions of reaction–diffusion equations in terms of functional integrals. We will not attempt to cover the general theory and all relevant equations. Our purpose is to discuss the main ideas and principal results and give illustrating examples involving typical equations. The reader interested in the general theory and all mathematical details will find a comprehensive treatment of the subject in Freidlin's book [141].

So far we have discussed the probabilistic solution of the convection–diffusion equation only. There are various directions in which a probabilistic approach to PDEs can be extended and generalized. The first direction is to extend it to the case where chemical reactions are taken into account. The next direction would be to allow the velocity field $\mathbf{v}$ and the diffusion matrix D to depend on both space $\mathbf{x}$ and time t. Another direction for generalization is to analyze initial-boundary problems.

3.7.4.1 Path-Integral and Feynman–Kac Formula

We start with the one-dimensional reaction–diffusion equation

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2} + r(x)\rho, \quad x \in \mathbb{R}, \tag{3.323}$$

where the function $r(x)$ represents the intrinsic growth rate. The solution to the reaction–diffusion equation (3.323) with $\rho(x,0) = \rho_0(x)$ can be written as the Feynman path integral, a functional integral,

$$\rho(x,t) = \int_{x(0)=x} \rho_0(x(t)) \exp\left\{ -\int_0^t \left[\frac{\dot{x}^2(s)}{4D} - r(x(s)) \right] \mathrm{d}s \right\} \mathcal{D}x(s), \tag{3.324}$$

where the integration is performed over all trajectories $x(s)$ starting at point x. The propagator, $p(y,t|x)$ can be written as

$$p(y,t|x) = \int_{\substack{x(0)=x \\ x(t)=y}} \exp\left\{ -\int_0^t \left[\frac{\dot{x}^2(s)}{4D} \right] \mathrm{d}s \right\} \mathcal{D}x(s), \tag{3.325}$$

which is the transition probability density function for the Brownian motion: $p(y,t|x) = \dfrac{\partial}{\partial y}\mathbb{P}(B(t) \le y | B(0) = x)$. So the path-integral (3.324) can be rewritten in terms of the expectation operator, the Feynman–Kac formula,

$$\rho(x,t) = \mathbb{E}_x \rho_0(B(t)) \exp\left(\int_0^t r(B(s))\mathrm{d}s \right), \tag{3.326}$$

where $B(t)$ is the Brownian motion starting at point x [141].

If the mesoscopic density of particles obeys the integro-differential equation

$$\frac{\partial \rho}{\partial t} = \lambda \int_{\mathbb{R}} \rho(x - z, t) w(z) \mathrm{d}z - \lambda \rho(x, t) + r(x)\rho, \tag{3.327}$$

then the underlying random process is a compound Poisson process $X(t)$ given by

$$X(t) = \sum_{i=1}^{N(t)} Z_i, \tag{3.328}$$

where $N(t)$ is a Poisson process with the transition rate λ and Z_i is a sequence of IID jumps with density function $w(z)$. The solution to the integro-differential equation (3.327) with the initial condition $\rho(x, 0) = \rho_0(x)$ can be written as

$$\rho(x, t) = \mathbb{E}_x \rho_0(X(t)) \exp\left(\int_0^t r(X(s)) \mathrm{d}s \right). \tag{3.329}$$

If the process $X(t)$ is a symmetric α-stable Lévy motion $S_\alpha(t)$ on $\mathbb{R}$, then the formula (3.329) provides the solution to the Cauchy problem

$$\frac{\partial \rho}{\partial t} = D_\alpha \frac{\partial^\alpha \rho}{\partial |x|^\alpha} + r(x)\rho, \quad \rho(x, 0) = \rho_0(x), \quad x \in \mathbb{R}. \tag{3.330}$$

In the same way we can obtain the probabilistic representation for the density that obeys the nonlinear Cauchy problem

$$\frac{\partial \rho}{\partial t} = D\Delta\rho + r(x, \rho)\rho, \quad \rho(\mathbf{x}, 0) = \rho_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3. \tag{3.331}$$

We have

$$\rho(\mathbf{x}, t) = \mathbb{E}_{\mathbf{x}} \rho_0(\mathbf{B}(t)) \exp\left[\int_0^t r(\mathbf{B}(s), \rho(\mathbf{B}(s), t - s) \mathrm{d}s \right]. \tag{3.332}$$

3.7.4.2 Nonstationary Convection–Diffusion Equation with Reactions

So far the velocity field $\mathbf{v}$ and the growth rate r have been functions of the space coordinate only. The goal now is to allow both $\mathbf{v}$ and r to depend on time t as well. Consider a transport problem involving a nonstationary incompressible fluid flow with the velocity field $\mathbf{v}(\mathbf{x}, t)$, standard diffusion with the constant diffusivity D, and reactions with rate $r(x, t)\rho$. The equation for the density of particles takes the form

$$\frac{\partial \rho}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla \rho = D\Delta\rho + r(\mathbf{x}, t)\rho, \quad \mathbf{x} \in \mathbb{R}^3, \tag{3.333}$$

with the initial condition

$$\rho(\mathbf{x}, t) = \rho_0(\mathbf{x}). \tag{3.334}$$

The solution of this problem can be written as the functional integral

$$\rho(\mathbf{x}, t) = \mathbb{E}_{\mathbf{x}} \rho_0(\mathbf{X}(t)) \exp\left[\int_0^t r(\mathbf{X}(s), t-s)\mathrm{d}s\right], \tag{3.335}$$

where the random process $\mathbf{X}(s)$ is the solution of the SDE

$$\mathrm{d}\mathbf{X}(s) = -\mathbf{v}(\mathbf{X}(s), t-s)\mathrm{d}s + \sqrt{2D}\mathrm{d}\mathbf{W}(s), \quad 0 \le s \le t, \tag{3.336}$$

with the initial condition $\mathbf{X}(0) = \mathbf{x}$. Here $\mathbf{W}(t)$ is the standard three-dimensional Wiener process.

In particular, the solution of the convection–diffusion equation ($r = 0$) is

$$\rho(\mathbf{x}, t) = \mathbb{E}_{\mathbf{x}} \rho_0(\mathbf{X}(t)). \tag{3.337}$$

In the next section we show why the velocity in (3.336) has arguments $(\mathbf{X}(s), t-s)$ and why there is a minus sign for this velocity.

3.7.4.3 Convection–Transport Equation

Consider a convection–transport equation without diffusion,

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla \rho(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \mathbb{R}^3, \tag{3.338}$$

with the initial condition $\rho(\mathbf{x}, 0) = \rho_0(\mathbf{x})$. The solution to this Cauchy problem can be written as follows:

$$\rho(\mathbf{x}, t) = \rho_0(\mathbf{X}(t)), \tag{3.339}$$

where $\mathbf{X}(t)$ is the solution of the characteristic equation

$$\mathrm{d}\mathbf{X}(s) = -\mathbf{v}(\mathbf{X}(s), t-s)\mathrm{d}s, \quad \mathbf{X}(0) = \mathbf{x}, \quad 0 \le s \le t. \tag{3.340}$$

The formula (3.339) tells us that the value of the density at point $\mathbf{x}$ at time t is the value of the initial density at the point $\mathbf{X}(t)$. The main idea is that we release the underlying process $\mathbf{X}(s)$ from the point $\mathbf{x}$ so that s varies from 0 up to t. So we allow the particle to move backward in time, such that the velocity field has a value $-\mathbf{v}(\mathbf{x}, t)$ at time $s = 0$ and $-\mathbf{v}(\mathbf{X}(t), 0)$ at time $s = t$. We have

$$\frac{\mathrm{d}\rho(\mathbf{X}(s), t-s)}{\mathrm{d}s} = \frac{\mathrm{d}\mathbf{X}(s)}{\mathrm{d}s} \cdot \nabla \rho(\mathbf{X}(s), t-s) - \frac{\partial \rho(\mathbf{X}(s), t-s)}{\partial t}. \tag{3.341}$$

We integrate both sides and find

$$\rho_0(\mathbf{X}(t)) - \rho(\mathbf{x}, t) = \\ -\int_0^t \left(\mathbf{v}(\mathbf{X}(s), t-s) \cdot \nabla \rho(\mathbf{X}(s), t-s) + \frac{\partial \rho(\mathbf{X}(s), t-s)}{\partial t} \right) \mathrm{d}s. \quad (3.342)$$

Because of (3.338) the RHS of the last equation is zero, and therefore $\rho(\mathbf{x}, t) = \rho_0(\mathbf{X}(t))$.

3.7.4.4 Boundary Reaction–Diffusion Problem

So far we have found probabilistic solutions to PDEs on the whole space. In fact Itô's formula allows us to represent the solutions to these equations in a bounded domain, $\Omega \in \mathbb{R}^3$, with appropriate boundary conditions. For example, let us consider the stationary reaction–diffusion problem

$$D\Delta\rho(\mathbf{x}) + r(\mathbf{x})\rho = 0, \quad \mathbf{x} \in \Omega, \quad \rho(\mathbf{x})_{\mathbf{x}\in\partial\Omega} = g(\mathbf{x}). \quad (3.343)$$

Then

$$\rho(\mathbf{x}) = \mathbb{E}_{\mathbf{x}} g(\mathbf{B}(\tau)) \exp\left\{ \int_0^\tau r(\mathbf{B}(s))\mathrm{d}s \right\}, \quad (3.344)$$

where $\mathbf{B}(t)$ is the Brownian motion starting at point $\mathbf{x}$ and τ is the first exit time for Brownian motion to reach the boundary $\partial\Omega$, i.e., $\tau = \min(t : \mathbf{B}(t) \notin \Omega)$. Freidlin's book [141] is an excellent reference for more details on initial-boundary problems similar to (3.343) and corresponding diffusion processes.

Exercises

3.1 Show that the Laplace transform of the Caputo derivative defined in (3.38) is

$$\mathcal{L}\left(\frac{\partial^\gamma p(x,t)}{\partial t^\gamma} \right) = s^\gamma \hat{p}(x,s) - s^{\gamma-1} p_0(x). \quad (3.345)$$

Hint: Use the definition of the Gamma function $\Gamma(1-\gamma) = \int_0^\infty \mathrm{e}^{-t} t^{-\gamma} \mathrm{d}t$ and the fact that the integral in (3.38) is the convolution of the functions $f(t)$ and $t^{-\gamma}$.

3.2 Using the Montroll–Weiss equation (3.31) for the uncoupled case (3.23), derive the equation for $\rho(x,t)$ in the form

$$\int_0^t M(t-\tau)\frac{\partial \rho(x,\tau)}{\partial \tau}\mathrm{d}\tau = \int_{\mathbb{R}} \rho(x-z,t)w(z)\mathrm{d}z - \rho(x,t), \tag{3.346}$$

where $M(t)$ is defined by its Laplace transform $\hat{M}(s) = [1-\hat{\phi}(s)]/[s\hat{\phi}(s)]$. Note that this is an alternative equation to the Master equation (3.31).

3.3 Obtain (3.141) from (3.139) and (3.140).

3.4 Assume that the waiting time PDF $\phi(t)$ corresponds to the family of Gamma distributions with parameters $m = 2$ and λ:

$$\phi(t) = \frac{\lambda^2 t \mathrm{e}^{-\lambda t}}{\Gamma(2)}. \tag{3.347}$$

If the kinetic term is linear, show that the solution to (3.130) is $\rho(x,t) = \mathrm{e}^{rt}n(x,t)$, where $n(x,t)$ is the solution to

$$\frac{1}{2\lambda}\frac{\partial^2 \rho}{\partial t^2} + \frac{\partial \rho}{\partial t} = \frac{\lambda}{2}\left[\int_{\mathbb{R}} \rho(x-z,\tau)w(z)\mathrm{d}z - \rho(x,\tau)\right]. \tag{3.348}$$

3.5 If the survival probability is

$$\Psi(t) = E_\gamma\left[-\left(\frac{t}{\tau_0}\right)^\gamma\right], \quad 0 < \gamma \leq 1, \tag{3.349}$$

where $E_\gamma[x] = \sum_0^\infty x^n/\Gamma(\gamma n + 1)$ is the Mittag–Leffler function, show that (3.130) can be written as the fractional reaction–transport equation

$$\begin{aligned}\frac{\partial \rho}{\partial t} = {} & \frac{\mathrm{e}^{\int_0^t f(\rho(x-z,u))\mathrm{d}u}}{\tau_0^\gamma}\mathcal{D}_t^{1-\gamma}\left(\int_{\mathbb{R}} \rho(x-z,t)\mathrm{e}^{-\int_0^t f(\rho(x-z,u))\mathrm{d}u}w(z)\mathrm{d}z\right) \\ & - \frac{\mathrm{e}^{\int_0^t f(\rho(x,u))\mathrm{d}u}}{\tau_0^\gamma}\mathcal{D}_t^{1-\gamma}\left(\rho(x,t)\mathrm{e}^{-\int_0^t f(\rho(x,u))\mathrm{d}u}\right) + f(\rho)\rho,\end{aligned} \tag{3.350}$$

where $\mathcal{D}_t^{1-\gamma}$ is the Riemann–Liouville fractional derivative defined by (2.58).