3. Stochastic processes

Next, we turn to the modeling of the evolution of stochastic variables. There are two ways to address this question. The first way is to describe the evolution of the PDF that characterizes a stochastic process. This approach will be described in the first three sections. A general transport equation for the PDF of a stochastic process will be derived in section 3.1. This equation will be simplified in section 3.2 to a Fokker-Planck equation. Section 3.3 deals with an example: it presents an exact solution to this Fokker-Planck equation. The second way to describe the evolution of stochastic processes is to postulate stochastic equations for them. Basics of this approach will be presented in section 3.4, and a more general (and more demanding) approach to solve this question is given in Appendix 3A. An essential element of this introduction of stochastic equations is the explanation of the relationships between processes that are described by stochastic differential equations and Fokker-Planck equations. Section 3.5 provides a link to the following chapters: it specifies the requirements for the construction of closed stochastic equations for any specific case considered.

3.1. PDF transport equations

3.1.1. The Kramers-Moyal equation

To prepare for the consideration of Fokker-Planck equations in section 3.2, we introduce first a general frame for PDF transport equations. For simplicity, we consider only one stochastic variable ξ. According to (2.4), its PDF is given by

$$F_{\xi}(x, t+\Delta t) = \langle \delta(x - \xi(t+\Delta t)) \rangle, \tag{3.1}$$

where Δt is a positive, infinitesimal time interval. To relate the right-hand side to the PDF at the previous time step $F_{\xi}(x, t)$, we expand the delta function into a Taylor series at $x - \xi(t)$,

$$\delta(x - \xi(t) + \xi(t) - \xi(t+\Delta t)) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n \delta(x - \xi(t))}{dx^n} [\xi(t) - \xi(t+\Delta t)]^n. \tag{3.2}$$

By inserting (3.2) into (3.1) we obtain

$$F_\xi(x, t+\Delta t) - F_\xi(x, t) = \sum_{n=1}^{\infty} \frac{1}{n!}\left(-\frac{d}{dx}\right)^n \left\langle [\xi(t+\Delta t) - \xi(t)]^n \delta(x - \xi(t)) \right\rangle, \qquad (3.3)$$

where the term of zeroth-order is written onto the left-hand side. We may now adopt (2.35) for conditional means to rewrite the right-hand side of (3.3) into

$$F_\xi(x, t+\Delta t) - F_\xi(x, t) = \sum_{n=1}^{\infty} \frac{1}{n!}\left(-\frac{d}{dx}\right)^n \left\langle [\xi(t+\Delta t) - \xi(t)]^n \,\middle|\, x, t \right\rangle F_\xi(x, t). \qquad (3.4)$$

The division of (3.4) by Δt and consideration of the limit $\Delta t \to 0$ then results in

$$\frac{\partial}{\partial t} F_\xi(x, t) = \sum_{n=1}^{\infty} \left(-\frac{\partial}{\partial x}\right)^n D^{(n)}(x, t)\, F_\xi(x, t), \qquad (3.5)$$

where the coefficients $D^{(n)}(x, t)$ are given by ($n \geq 1$)

$$D^{(n)}(x, t) = \lim_{\Delta t \to 0} \frac{1}{\Delta t\, n!} \left\langle [\xi(t+\Delta t) - \xi(t)]^n \,\middle|\, x, t \right\rangle. \qquad (3.6)$$

Equation (3.5) is called the Kramers-Moyal equation (Kramers 1940, Moyal 1949). It may be seen as the most general form of a PDF transport equation (if it is written for the case of a vector of several variables).

3.1.2. Markov processes

The difference $\Delta\xi = \xi(t + \Delta t) - \xi(t)$ in the coefficients (3.6) may depend on all the values of the stochastic variable ξ at earlier times, this means on $\xi(t - k\,\Delta t)$ with $k = 0, 1, \cdots$. However, very often one finds that the influence of such memory effects becomes negligible after a characteristic relaxation time. Thus, if we choose Δt such that it is large compared to this relaxation time of memory effects, we find that $\Delta\xi$ is fully determined by the state $\xi(t)$ (which is correlated to $\xi(t)$ in the difference $\Delta\xi$) and independent of states at earlier times. This assumption is found to be a good approximation under many circumstances provided a suitable set of stochastic variables is chosen; see for instance the detailed discussion of this question regarding the construction of stochastic velocity models in chapter 5.

Stochastic processes for which $\Delta\xi$ only depends on the state $\xi(t)$ are referred to as Markov processes (Gardiner 1983; Risken 1984). They will be considered now, which makes the general PDF transport equation (3.5) to an applicable tool for the investigation of the evolution of stochastic processes. In this case, the coefficients $D^{(n)}(x, t)$ depend only on x and t. Equation (3.5) represents then with respect to time t a differential equation of first-order. Combined with appropriate boundary conditions and the specification of an initial PDF $F_\xi(x, t_0)$, equation (3.5) uniquely determines the PDF $F_\xi(x, t)$.

3.1.3. Implications for PDF transport equations

To solve equation (3.5), one needs knowledge about the number of terms on the right-hand side that have to be considered. Regarding this, an important constraint arises from the theorem of Pawula (1967). This theorem may be shown by considering the implications of Schwarz's unequality (2.30), which also applies to conditional means (all the arguments given in section 2.3.2 may be repeated for the sample space considered). By choosing $\varphi = (\Delta\xi)^k$ and $\psi = (\Delta\xi)^{k+m}$, where $k \geq 1$ and $m \geq 1$, Schwarz's unequality implies for the coefficients (3.6) that

$$\left[(2k+m)!\, D^{(2k+m)}\right]^2 \leq (2k)!(2k+2m)!\, D^{(2k)}\ D^{(2k+2m)}. \tag{3.7}$$

First, we assume that $D^{(2k)} = 0$. This implies according to relation (3.7) that $D^{(2k+m)} = 0$; this means all the higher-order coefficients have to vanish. Second, we assume that $D^{(2k+2m)} = 0$. Relation (3.7) then implies that $D^{(2k+2m-m)} = 0$; this means all the lower-order coefficients have to vanish then (with the exception of $D^{(1)}$ and $D^{(2)}$ because $2k + m$ is bounded from below by 3). These two cases can be combined to produce the following result

$$D^{(2n)} = 0 \quad \rightarrow \quad D^{(3)} = D^{(4)} = \cdots = D^{(\infty)} = 0 \quad (n \geq 1). \tag{3.8}$$

Hence, $D^{(1)}$ may be zero or nonzero, this does not imply any restrictions. If we take $D^{(2)} = 0$, we have to restrict the series in (3.5) to the first term. If we take $D^{(2)} \neq 0$, we have two possibilities: we may consider only the first two terms in equation (3.5), or we have to involve an infinite number of nonzero coefficients of even order. We see therefore that the theorem of Pawula (1967) is very similar to the theorem of Marcienkiewicz (1939), see section 2.2.2. Both theorems make use of the definition of PDFs as positive definite quantities, i.e., PDFs may have negative values if the requirements of these theorems are not satisfied.

The consideration of an infinite number of coefficients of even order leads to the notable problems of providing all these coefficients as functions of the sample space variable x, and of solving such an equation numerically. Thus, the neglect of these coefficients $D^{(m)}$ ($m = 3, 4, \cdots$) seems to be the better way in general. However, this leads to the question under which conditions this is justified. The answer is closely related to the consideration of the continuity of the sample path of stochastic processes. By considering an infinitesimal time increment Δt, one can often expect that the change $\Delta\xi = \xi(t + \Delta t) - \xi(t)$ of a stochastic variable is bounded (i.e., small). Such stochastic processes have a continuous sample path, and one can show that the assumption of such a process implies the neglect of $D^{(m)}$ ($m = 3, 4, \cdots$), see Gardiner (1983). In other words, one takes jump processes into account (instantaneous changes $\Delta\xi$ that may be very large) which imply discontinuous sample paths if coefficients $D^{(m)}$ ($m = 3, 4, \cdots$) are involved. To exclude this case, we will neglect coefficients of higher than second order from now.

3.2. The Fokker-Planck equation

3.2.1. The Fokker-Planck equation

We consider a vectorial stochastic process $\boldsymbol{\xi} = \{\xi_1(t), \xi_2(t), \cdots, \xi_N(t)\}$ which is assumed to be Markovian and to have continuous sample paths. The corresponding extension of equation (3.5) reads

$$\frac{\partial}{\partial t} F_\xi(\mathbf{x},t) = -\frac{\partial}{\partial x_i} D_i(\mathbf{x},t)\, F_\xi(\mathbf{x},t) + \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}(\mathbf{x},t)\, F_\xi(\mathbf{x},t). \tag{3.9}$$

This equation is called a Fokker-Planck equation (Fokker 1914, Planck 1917). Its coefficients D_i and D_{ij} are given by the vectorial generalizations of $D^{(1)}$ and $D^{(2)}$,

$$D_i(\mathbf{x},t) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \left\langle \xi_i(t+\Delta t) - \xi_i(t) \,\middle|\, \mathbf{x}, t \right\rangle, \tag{3.10a}$$

$$D_{ij}(\mathbf{x},t) = \lim_{\Delta t \to 0} \frac{1}{2\Delta t} \left\langle \left[\xi_i(t+\Delta t) - \xi_i(t)\right] \left[\xi_j(t+\Delta t) - \xi_j(t)\right] \,\middle|\, \mathbf{x}, t \right\rangle. \tag{3.10b}$$

The conditional means refer to the condition $\boldsymbol{\xi}(t) = \mathbf{x}$. D_i may be seen as a generalized velocity if $\mathbf{x}$ is interpreted as generalized coordinate in sample space. Equation (3.9) corresponds then to a diffusion equation with D_{ij} as diffusion coefficient. Important properties of D_{ij} are that D_{ij} is symmetric and semidefinite. The latter may be seen by multiplying (3.10b) with any vectors c_i and c_j,

$$D_{ij} c_i c_j = \lim_{\Delta t \to 0} \frac{1}{2\Delta t} \left\langle \left\{ \left[\xi_i(t+\Delta t) - \xi_i(t)\right] c_i \right\}^2 \,\middle|\, \mathbf{x}, t \right\rangle \geq 0. \tag{3.11}$$

Usually, we will assume that D_{ij} is positive definite, $D_{ij}\, c_i\, c_j > 0$ for $c_i\, c_i > 0$. The inverse matrix of D_{ij} exists in this case.

To prove the consistency of (3.9), we integrate it over the sample space $\mathbf{x}$,

$$\frac{\partial}{\partial t} \int d\mathbf{x}\; F_\xi(\mathbf{x},t) = -\int d\mathbf{x}\; \frac{\partial}{\partial x_i} D_i(\mathbf{x},t) F_\xi(\mathbf{x},t) + \int d\mathbf{x}\; \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}(\mathbf{x},t) F_\xi(\mathbf{x},t)\,. \tag{3.12}$$

The left-hand side of (3.12) vanishes (F_ξ is assumed to be normalized to unity). By setting $D_i\ F_\xi$ and $\partial(D_{ij}\ F_\xi)\ /\ \partial x_j$ equal to L, respectively, the integrals on the right-hand side may be written as volume integrals over derivatives of L. The latter can be rewritten as surface integrals,

$$\int d\mathbf{x}\, \frac{\partial L}{\partial x_i} = \int_s ds\ L\ \mathbf{n}\, \boldsymbol{\eta}_i. \tag{3.13}$$

Here, s is the surface that surrounds the domain considered, and ds is a differential element of s. The unit vector of the x_i-axis is referred to by $\boldsymbol{\eta}_i$, and $\mathbf{n}$ is the normal vector of s. By considering an infinite domain, the integrals on the right-hand side of (3.13) will vanish if L is zero at the surface. Therefore, the consistency of the formulation of equation (3.9) requires the assumption that the PDF F_ξ and its derivatives vanish at $|\mathbf{x}| \rightarrow \infty$.

3.2.2. Transport equations for moments

The implications of equation (3.9) for the transport of moments of the PDF F_ξ will be considered next. By multiplying this equation with x_k and integration over the sample space we obtain

$$\frac{\partial}{\partial t}\langle \xi_k \rangle = -\int d\mathbf{x}\ x_k \frac{\partial}{\partial x_i} D_i(\mathbf{x},t) F_\xi(\mathbf{x},t) + \int d\mathbf{x}\ x_k \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}(\mathbf{x},t) F_\xi(\mathbf{x},t). \tag{3.14}$$

As done before, we set $D_i\ F_\xi$ and $\partial(D_{ij}\ F_\xi)\ /\ \partial x_j$ equal to L, respectively. The integrals of (3.14) may be rewritten then by adopting partial integration,

$$\int d\mathbf{x}\, \frac{\partial x_k L}{\partial x_i} = \delta_{ki} \int d\mathbf{x}\ L + \int d\mathbf{x}\ x_k \frac{\partial L}{\partial x_i}. \tag{3.15}$$

According to (3.13), combined with the assumption L = 0 at $|\mathbf{x}| \rightarrow \infty$, the left-hand side of (3.15) vanishes. By adopting the resulting relation in (3.14) we then obtain

$$\frac{\partial}{\partial t}\langle \xi_k \rangle = \langle D_k \rangle = \int d\mathbf{x}\ D_k(\mathbf{x},t) F_\xi(\mathbf{x},t) \tag{3.16}$$

since the last integral in (3.14) does not contribute. Hence, $\langle D_k \rangle$ determines the transport of the means $\langle \xi_k \rangle$. For that reason, D_k is called a drift coefficient.

In analogy to the derivation of (3.16), one may obtain the following relation for second-order moments by multiplication of (3.9) with $x_k\ x_n$ and integrating it over the sample space,

$$\frac{\partial}{\partial t}\langle \xi_k \xi_n \rangle = \langle D_k \xi_n \rangle + \langle D_n \xi_k \rangle + 2\langle D_{kn} \rangle. \tag{3.17}$$

To obtain this relation, partial integration has to be applied twice in accordance with (3.15). The combination of (3.16) and (3.17) can be used then to derive a transport equation for the variance

$$\langle \xi'_k \, \xi'_n \rangle = \langle (\xi_k - \langle \xi_k \rangle)(\xi_n - \langle \xi_n \rangle) \rangle = \langle \xi_k \xi_n \rangle - \langle \xi_k \rangle \langle \xi_n \rangle. \tag{3.18}$$

This variance transport equation reads

$$\frac{\partial}{\partial t} \langle \xi'_k \, \xi'_n \rangle = \langle D'_k \, \xi'_n \rangle + \langle D'_n \, \xi'_k \rangle + 2 \langle D_{kn} \rangle, \tag{3.19}$$

where $D'_k = D_k - <D_k>$ is written for fluctuations of D_k. Hence, variances are produced by $<D_{kn}>$ provided that D_{kn} is positive definite. The appearance of D_{kn} causes a diffusion process (the width of the PDF increases), which is the reason for the consideration of D_{kn} as a diffusion coefficient. An equilibrium state may be reached asymptotically if the first two terms on the right-hand side of (3.19) appear with a negative sign, i.e., if they are able to balance the variance production. These two terms then describe the dissipation (or destruction) of variance.

3.2.3. The limiting PDF

An important question concerns the conditions for the existence of a unique asymptotic state. To clarify this, we have to consider the asymptotic features of the PDF F_ξ that obeys the Fokker-Planck equation (3.9). As done by Lebowitz & Bergmann (1957) and Risken (1984), we consider an infinite domain and define the entropy difference related to two solutions $F_1(\mathbf{x}, t)$ and $F_2(\mathbf{x}, t)$ of the Fokker-Planck equation (3.9) (which may result from different initial PDFs) according to the entropy definition (2.42) by

$$h(t) = S_2(t) - S_1(t) = \left\langle \ln\left(\frac{F_1}{F_2}\right) \right\rangle = \int d\mathbf{x} \; F_1(\mathbf{x}, t) \ln\left(\frac{F_1(\mathbf{x}, t)}{F_2(\mathbf{x}, t)}\right). \tag{3.20}$$

The purpose of the following explanations is to show that $h(t) \geq 0$ and $dh / dt \leq 0$, this means h evolves towards $h = 0$. This limit $h = 0$ corresponds then to the asymptotic agreement of both solutions.

To show $h(t) \geq 0$, we rewrite relation (3.20) by adopting the normalization constraints for F_1 and F_2,

$$h(t) = \int d\mathbf{x} \; [F_1 \ln(R) - F_1 + F_2] = \int d\mathbf{x} \; F_2 \, g(R), \tag{3.21}$$

where the abbreviations $R = F_1 / F_2$ and $g(R) = R \ln(R) - R + 1$ are introduced. The analysis of the function $g(R)$ reveals that it takes its minimum zero at $R = 1$. Consequently, we find that $h(t)$ always has to be non-negative.

To show $dh / dt \le 0$, we calculate the derivative of $h(t)$,

$$\frac{dh}{dt}(t) = \int d\mathbf{x} \left[\frac{\partial F_1}{\partial t} \ln(R) + \frac{\partial F_1}{\partial t} - R \frac{\partial F_2}{\partial t} \right] = \int d\mathbf{x} \left[\frac{\partial F_1}{\partial t} \ln(R) - R \frac{\partial F_2}{\partial t} \right]. \tag{3.22}$$

The last expression arises from the fact that the integral over $\partial F_1 / \partial t$ has to vanish due to the normalization constraint. By adopting (3.9) to replace in equation (3.22) the derivatives of F_1 and F_2, we obtain

$$\frac{dh}{dt}(t) = -\int d\mathbf{x} \left\{ \ln(R) \frac{\partial}{\partial x_i} \left[D_i F_1 - \frac{\partial D_{ij} F_1}{\partial x_j} \right] - R \frac{\partial}{\partial x_i} \left[D_i F_2 - \frac{\partial D_{ij} F_2}{\partial x_j} \right] \right\}. \tag{3.23}$$

This expression may be rewritten by means of partial integration. We consider integrals over derivatives $\partial / \partial x_i$ in correspondence to relation (3.15), rewrite them according to (3.13), and assume that the integrands vanish at $|\mathbf{x}| \to \infty$. This leads to

$$\frac{dh}{dt}(t) = -\int d\mathbf{x} \left\{ \frac{\partial \ln(R)}{\partial x_i} \left[- D_i F_1 + \frac{\partial D_{ij} F_1}{\partial x_j} \right] - \frac{\partial R}{\partial x_i} \left[- D_i F_2 + \frac{\partial D_{ij} F_2}{\partial x_j} \right] \right\}. \tag{3.24}$$

This relation reduces to

$$\frac{dh}{dt}(t) = -\int d\mathbf{x} \left\{ \frac{\partial \ln(R)}{\partial x_i} \frac{\partial D_{ij} F_1}{\partial x_j} - \frac{\partial R}{\partial x_i} \frac{\partial D_{ij} F_2}{\partial x_j} \right\} \tag{3.25}$$

because the terms that involve D_i cancel each other. The latter may be seen by rewriting the derivative of $\ln(R)$ into a derivative of R. We replace F_2 by F_1 / R and apply partial integration to obtain

$$\frac{dh}{dt}(t) = -\int d\mathbf{x}\ D_{ij} F_1 \left\{ \frac{1}{R} \frac{\partial^2 R}{\partial x_j \partial x_i} - \frac{\partial^2 \ln(R)}{\partial x_i \partial x_j} \right\}. \tag{3.26}$$

The first term within the bracket on the right-hand side may be rewritten by means of the relation $\partial R / \partial x_i = R\, \partial \ln(R) / \partial x_i$. This leads then to

$$\frac{dh}{dt}(t) = -\int d\mathbf{x}\ D_{ij} F_1 \frac{\partial \ln(R)}{\partial x_j} \frac{\partial \ln(R)}{\partial x_i}. \tag{3.27}$$

Hence, $dh / dt \le 0$ if D_{ij} is positive definite. This means, h will evolve towards its minimum $h = 0$ provided D_i and D_{ij} have no singularities and do not permit that infinite values of solutions of (3.9) appear at $|\mathbf{x}| \to \infty$. For $h = 0$, different solutions of the Fokker-Planck equation have to coincide such that $F_1 = F_2$. This unique asymptotic solution is the stationary solution of (3.9) for the case that D_i and D_{ij} are independent of time.

To show the relation of these conclusions to the consideration of the entropy in chapter 2, we consider a special case. We assume that the limiting PDF was chosen to be the initial PDF of F_2, so that F_2 will not change in time. h(t) is then the positive difference of the entropies related to the limiting PDF F_2 and F_1, respectively. The fact that h evolves towards its minimum h = 0 describes the increase of entropy of a system for which a limiting state exists. The entropy will become maximal if this limiting state is reached. Due to the disappearance of the left-hand side, the Fokker-Planck equation (3.9) implies in the equilibrium case

$$\frac{\partial \ln\left(F_\xi\right)}{\partial x_j} = D^{-1}{}_{jk}\left(D_k - \frac{\partial D_{kj}}{\partial x_j} \right). \tag{3.28}$$

This expression is consistent with the structure of SML PDFs considered in chapter 2: the choice of D_k as a polynomial of n^{th}-order corresponds to the specification of a SML PDF of n^{th}-order.

3.3. An exact solution to the Fokker-Planck equation

3.3.1. The equation considered

To illustrate the application of Fokker-Planck equations and characteristics of their solutions, let us consider an example that enables the derivation of analytical results. In conjunction with the assumption of natural boundary conditions (this means $F_\xi(\mathbf{x}, t) \to 0$ for $|\mathbf{x}| \to \infty$), we specify the Fokker-Planck equation (3.9) in the following way,

$$\frac{\partial}{\partial t} F_\xi(\mathbf{x}, t) = -\frac{\partial}{\partial x_i}\left[G_i(t) + G_{ik}(t)\left\{ x_k - \langle \xi_k \rangle \right\} \right] F_\xi(\mathbf{x}, t) + \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}(t)\, F_\xi(\mathbf{x}, t). \tag{3.29}$$

The drift coefficient D_i is written as a linear function of the variables $\mathbf{x}$, which may be seen as the Taylor series of D_i in the first order of approximation. The inclusion of $<\xi_k>$ in (3.29) defines G_{ik} as the coefficient that controls the intensity of fluctuations around the mean $<\xi_k>$. It will be shown in the following chapters that such linear models for D_i are well suited to characterize near-equilibrium processes. The diffusion coefficient D_{ij} is assumed to be only a function of time. This choice is convenient with regard to many applications, see the explanations given in the following chapters. In addition to this, one can guarantee in this way the important property of D_{ij} to be semidefinite.

3.3.2. The solution to the Fokker-Planck equation

The solution to the Fokker-Planck equation (3.29) depends on the initial PDF $F_\xi(\mathbf{x}', t')$ according to relation (2.32),

$$F_\xi(\mathbf{x}, t) = \int d\mathbf{x}' \, F_{\xi|\xi}(\mathbf{x}, t \,|\, \mathbf{x}', t') \, F_\xi(\mathbf{x}', t'). \tag{3.30}$$

Therefore, to obtain a general solution to equation (3.29) one has to calculate the conditional PDF $F_{\xi|\xi}$. Specific solutions $F_\xi(\mathbf{x}, t)$ can be obtained then in dependence on specified initial PDFs $F_\xi(\mathbf{x}', t')$ by integration according to (3.30). By inserting relation (3.30) into equation (3.29) one may prove that the conditional PDF $F_{\xi|\xi}$ also satisfies the Fokker-Planck equation (3.29). According to (2.37), the required initial condition for $F_{\xi|\xi}$ is given by

$$F_{\xi|\xi}(\mathbf{x}', t' \,|\, \mathbf{x}', t') = \delta(\mathbf{x} - \mathbf{x}'). \tag{3.31}$$

The coefficients in (3.29) are specified as linear functions of the sample space variables $\mathbf{x}$. Thus, one may assume that the PDF evolves towards a Gaussian shape. To prove this idea, we consider the conditional PDF $F_{\xi|\xi}$ as a N-dimensional Gaussian PDF,

$$F_{\xi|\xi}(\mathbf{x}, t \,|\, \mathbf{x}', t') = \frac{1}{(2\pi)^{N/2}\sqrt{\det(\alpha)}} \exp\left\{-\frac{1}{2}\alpha^{-1}{}_{kl}(x_k - \alpha_k)(x_l - \alpha_l)\right\}. \tag{3.32}$$

The means of this PDF are given by α_k, the variances by α_{kl}, and $\det(\alpha)$ is the determinant of the matrix α with the elements α_{kl}. What one has to do now is to explain the relationship between α_k and α_{kl} with the coefficients G_i, G_{ik}, and D_{ij} of the Fokker-Planck equation (3.29). To do this, we calculate the corresponding derivatives of (3.32) and insert them into (3.29). This leads to three conditions for the coefficients of terms of zeroth-, first- and second-order in the variables considered. One condition is satisfied identically, and the other two constraints lead to the following equations for the means α_k and variances α_{kl} of (3.32),

$$\frac{\partial \alpha_k}{\partial t} = G_k + G_{kn}(\alpha_n - \langle \xi_n \rangle), \tag{3.33a}$$

$$\frac{\partial \alpha_{kl}}{\partial t} = G_{kn}\alpha_{nl} + G_{ln}\alpha_{nk} + 2D_{kl}. \tag{3.33b}$$

To derive (3.33a-b) we applied the following relations for the variances α_{kl},

$$\frac{1}{\det(\alpha)}\frac{\partial \det(\alpha)}{\partial t} = -\frac{\partial \alpha^{-1}{}_{mn}}{\partial t}\alpha_{nm}, \qquad \frac{\partial \alpha^{-1}{}_{mn}}{\partial t} = -\alpha^{-1}{}_{mk}\frac{\partial \alpha_{kl}}{\partial t}\alpha^{-1}{}_{ln}. \tag{3.34}$$

The first relation of (3.34) may be obtained by the differentiation of (3.32) by time and integration over the sample space. The second relation can be derived by the differentiation of the identity $\alpha_{in}\,\alpha^{-1}_{nj} = \delta_{ij}$. Hence, we find that (3.32) provides the solution to (3.29) provided the means α_k and variances α_{kl} satisfy (3.33a-b). The initial conditions for these equations (3.33a-b) are given by

$$\alpha_k(t') = x'_k\,, \tag{3.35a}$$

$$\alpha_{kl}(t') = 0. \tag{3.35b}$$

By adopting the properties of delta functions, one may prove that (3.32) combined with (3.35a-b) recovers the initial condition (3.31) for the conditional PDF $F_{\xi|\xi}$.

3.3.3. Means, variances and correlations

Next, let us have a look at the means and variances of $F_\xi(\mathbf{x}, t)$, which are implied by the Fokker-Planck equation (3.29). One way to obtain these quantities is to derive them from expression (3.30) for the PDF $F_\xi(\mathbf{x}, t)$ in combination with (3.32) for the conditional PDF $F_{\xi|\xi}$. However, this approach requires the specification of the initial PDF $F_\xi(\mathbf{x}', t')$ and integration of the transport equations (3.33a-b) for α_k and α_{kl}. A simpler way is to derive directly transport equations for the means and variances of $F_\xi(\mathbf{x}, t)$, as pointed out in section 3.2.2. In this way, we find the equations

$$\frac{\partial\langle\xi_k\rangle}{\partial t} = G_k\,, \tag{3.36a}$$

$$\frac{\partial\langle\xi'_k\,\xi'_l\rangle}{\partial t} = G_{kn}\langle\xi'_n\,\xi'_l\rangle + G_{ln}\langle\xi'_n\,\xi'_k\rangle + 2D_{kl}\,, \tag{3.36b}$$

which have to be solved in conjunction with the corresponding initial conditions provided by the initial PDF.

The equations (3.36a-b) can be used to rewrite the equations (3.33a-b) for α_k and α_{kl}. The combination of these equations leads to

$$\frac{\partial}{\partial t}\big(\alpha_k - \langle\xi_k\rangle\big) = G_{kn}\big(\alpha_n - \langle\xi_n\rangle\big), \tag{3.37a}$$

$$\frac{\partial}{\partial t}\big(\alpha_{kl} - \langle\xi'_k\,\xi'_l\rangle\big) = G_{kn}\big(\alpha_{nl} - \langle\xi'_n\,\xi'_l\rangle\big) + G_{ln}\big(\alpha_{nk} - \langle\xi'_n\,\xi'_k\rangle\big). \tag{3.37b}$$

These equations show that α_k and α_{kl} relax to the means and variances of $F_\xi(\mathbf{x}, t)$. Asymptotically, the left hand sides of (3.37a-b) vanish, and α_k and α_{kl} become equal to the means and variances of $F_\xi(x, t)$,

$$\alpha_k = \langle \xi_k \rangle, \tag{3.38a}$$

$$\alpha_{kl} = \langle \xi'_k \, \xi'_l \rangle. \tag{3.38b}$$

In this case, the conditional PDF is independent of **x'**, as may be seen by adopting (3.38a-b) in the parametrization (3.32) for $F_{\xi|\xi}$. Equation (3.30) reveals then that the PDF F_ξ is equal to the conditional PDF $F_{\xi|\xi}$. Accordingly, the unconditional PDF F_ξ and conditional PDF $F_{\xi|\xi}$ relax asymptotically (independent of the initial conditions) to a Gaussian function.

Another relevant characteristics of the Fokker-Planck equation (3.29) is the two-point correlation function, which is defined by ($s \geq 0$)

$$\langle \xi'_k(t) \, \xi'_l(t+s) \rangle = \int d\mathbf{x} \, d\mathbf{x'} \left(x_k - \langle \xi_k(t) \rangle \right) \left(x'_l - \langle \xi_l(t+s) \rangle \right) F_{\xi\xi}(\mathbf{x}, t; \mathbf{x'}, t+s). \tag{3.39}$$

The two-point PDF $F_{\xi\xi}$ has also to satisfy equation (3.29), as may be seen by means of the definition (2.31) of the two-point PDF. The integration of (3.29) multiplied with the corresponding variables results then in the following equation for the correlation function,

$$\frac{\partial}{\partial s} \langle \xi'_k(t) \, \xi'_l(t+s) \rangle = G_{km} \langle \xi'_m(t) \, \xi'_l(t+s) \rangle. \tag{3.40}$$

The initial condition is given by the variance of $F_\xi(\mathbf{x}, t)$ at t. Accordingly, the correlation decays exponentially for the dynamics considered: the memory lost is controlled by $-G_{km}$, which represents a frequency (inverse time scale) matrix. In contrast to the evolution of variances, which is determined by equation (3.36b), there is no production mechanism for correlations (provided that $-G_{km}$ is non-negative as usually assumed): memory can only be lost.

3.4. Stochastic equations for realizations

One way to model the evolution of stochastic variables was considered in the previous three sections, where equations for the PDF of stochastic variables were introduced. It was argued that the reduction of the Kramers-Moyal equation (3.5) (written for the case of several variables) to the Fokker-Planck equation (3.9) has to be seen as the most suitable way of constructing a PDF transport equation. An alternative approach is to postulate differential equations for the calculation of the evolution of stochastic variables. The stochastic processes determined in this way can then be applied to calculate all the coefficients of the Kramers-Moyal equation, this means this approach results, too, in a specific PDF transport equation. The relations between these two approaches will be considered next.

3.4.1. Stochastic differential equations

A general evolution equation for a vector $\xi(t) = \{\xi_1(t), \xi_2(t), \cdots, \xi_N(t)\}$ of N stochastic variables may be written in the following way ($0 \leq s \leq t$),

$$\frac{d\xi_i}{dt} = a_i[\xi(s), s] + f_i. \tag{3.41}$$

f_i represents any stochastic force which produces fluctuations of ξ. We assume that f_i vanishes in the ensemble average, and that it has a characteristic correlation time τ_f (fluctuations of f_i are relaxed, basically, after the time τ_f). Usually, a_i represents the dynamics of mean values of ξ and the relaxation of fluctuations of ξ. This term is a deterministic functional that may depend on all states $\xi(s)$ at earlier times (which makes ξ to a non-Markovian process, see section 3.1.2).

Obviously, the consideration of memory effects in a_i and a finite correlation time τ_f of stochastic forces may hamper analyses and applications of (3.41) significantly. A very important experience is that a suitable choice of variables often enables the consideration the characteristic relaxation time τ_f of f_i as infinitely small compared to the typical time scales of the problem considered (this may require, for instance, the extension of the set of variables considered by constructing models that include equations for derivatives of ξ, see the explanations given in Appendix 3A and chapter 5). In this case, the stochastic forces in (3.41) can be seen to be uncorrelated and the influence of memory effects on a_i can be neglected (the close relation between stochastic force correlations and memory effects is pointed out in detail in Appendix 3A). This assumption of vanishing memory effects and correlation times τ_f will be made now, this means we restrict the attention to the consideration of the equation

$$\frac{d\xi_i}{dt} = a_i(\xi, t) + b_{ik}(\xi, t)\frac{dW_k}{dt}. \tag{3.42}$$

In this equation, a_i and b_{ik} are any deterministic functions of $\xi(t)$ and t. The stochastic process dW_k / dt represents the derivative of the k^{th} component of a vectorial Gaussian process $\mathbf{W} = (W_1, \cdots, W_N)$, which is called a Wiener process (Gardiner 1983, Risken 1984). Hence, dW_k / dt is fully determined by its first two moments that are given by

$$\left\langle \frac{dW_k}{dt} \right\rangle = 0, \tag{3.43a}$$

$$\left\langle \frac{dW_k}{dt}(t)\frac{dW_l}{dt}(t') \right\rangle = \delta_{kl}\delta(t - t'). \tag{3.43b}$$

In accord with the assumed properties of the stochastic force f_i, the relations (3.43a-b) mean that f_i vanishes in the ensemble average, and that its correlation time is zero (it is uncorrelated for different times). In addition to this, it is assumed that there are no correlations between different stochastic force components. Hence, the change of ξ_i modeled by (3.42) is completely determined by the state of $\boldsymbol{\xi}$ at t, such that $\boldsymbol{\xi}(t)$ represents a Markov process.

It is essential to note that (in contrast to the integration of ordinary differential equations) the value of integrals that involve stochastic variables may depend on the definition of the integration. Throughout this book we will use the Itô-definition for this (Gardiner 1983, Risken 1984). The latter assumes that the formal solution of the equation (3.42) is given by

$$\begin{aligned}\xi_i(t+\Delta t)-\xi_i(t) &= \int_t^{t+\Delta t} ds\; a_i(\boldsymbol{\xi}(s),s) + \int_t^{t+\Delta t} ds\; b_{ik}(\boldsymbol{\xi}(s),s)\frac{dW_k}{ds}(s) \\ &= a_i(\boldsymbol{\xi}(t),t)\,\Delta t + b_{ik}(\boldsymbol{\xi}(t),t)\,\Delta W_k(t), \end{aligned} \tag{3.44}$$

where Δt is an infinitesimal time increment. The assumption related to the second line of equation (3.44) is that the coefficients a_i and b_{ik} in the integrals are taken at the previous time step t. Further, we introduced the variable

$$\Delta W_k(t) = \int_t^{t+\Delta t} ds\; \frac{dW_k}{ds}(s) = W_k(t+\Delta t) - W_k(t). \tag{3.45}$$

By adopting the properties (3.43a-b) of $dW_k\, /\, dt$, the properties of the Gaussian process ΔW_k are found to be

$$\langle \Delta W_k(t) \rangle = 0, \tag{3.46a}$$

$$\begin{aligned}\langle \Delta W_k(t)\,\Delta W_l(t') \rangle &= \int_t^{t+\Delta t} ds \int_{t'}^{t'+\Delta t} ds' \left\langle \frac{dW_k}{ds}(s)\frac{dW_l}{ds'}(s') \right\rangle = \delta_{kl} \int_t^{t+\Delta t} ds \int_{t'}^{t'+\Delta t} ds'\; \delta(s'-s) \\ &= \delta_{kl} \int_t^{t+\Delta t} ds\; [\theta(t'+\Delta t - s) - \theta(t'-s)] = (1-k)\Delta t\, \delta_{kl}, \end{aligned} \tag{3.46b}$$

where $t' = t - k\,\Delta t$ ($k = 0, 1$) is applied as an abbreviation. Therefore, the values of ΔW_k at the same time step ($k = 0$) are correlated, whereas values at different times ($k = 1$) are uncorrelated (obviously, $\Delta W_k(t)$ is also uncorrelated to $\Delta W_k(t')$ with $k = 2, 3, \cdots$). Two examples for realizations of ΔW_k normalized to $(\Delta t)^{1/2}$ are shown in Fig. 3.1. This figure reveals that there is no correlation between adjacent values and various realizations. According to the relations (3.46a-b), these standardized numbers have a zero mean and a variance equal to unity.

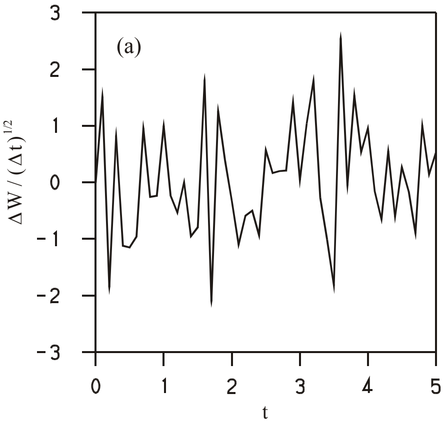

Fig. 3.1. Two examples for realizations of one component of $\Delta W / (\Delta t)^{1/2}$.

According to its definition (3.45), $\Delta W_k / \Delta t$ represents the derivative of W_k. By dividing (3.46b) by $(\Delta t)^2$, we see that the variance of $\Delta W_k / \Delta t$ does not exist: it diverges proportional to $(\Delta t)^{-1/2}$, this means it goes to infinity for $\Delta t \to 0$. Consequently, W_k is not differentiable because the probability for the appearance of $\Delta W_k / \Delta t$ values that are larger than any limit is equal to unity (Gardiner 1983). For that reason, stochastic equations are often written according to the formulation (3.44) where ΔW_k behaves properly. Nevertheless, the equation (3.42) will be used here in general to represent stochastic equations, having in mind that it states nothing else than the formulation (3.44).

3.4.2. The relationship to Fokker-Planck equations

Equation (3.42) determines the evolution of the stochastic process $\boldsymbol{\xi}$. Consequently, it has to imply a PDF transport equation. This fact leads then to the question about the relation of the PDF transport equation implied by (3.42) to the Fokker-Planck equation (3.9). To address this, we calculate the first two coefficients of the Kramers-Moyal equation (written for the case of several variables), which are equal to the coefficient D_i and D_{ij} of the Fokker-Planck equation (3.9). By inserting (3.44) into (3.10a-b) we find

$$D_i(\mathbf{x},t) = a_i(\mathbf{x},t), \tag{3.47a}$$

$$D_{ij}(\mathbf{x},t) = \frac{1}{2} b_{ik}(\mathbf{x},t)\, b_{jk}(\mathbf{x},t). \tag{3.47b}$$

where the properties (3.46a-b) of ΔW_k are used. The corresponding calculation of higher-order coefficients of the Kramers-Moyal equation reveals that all these

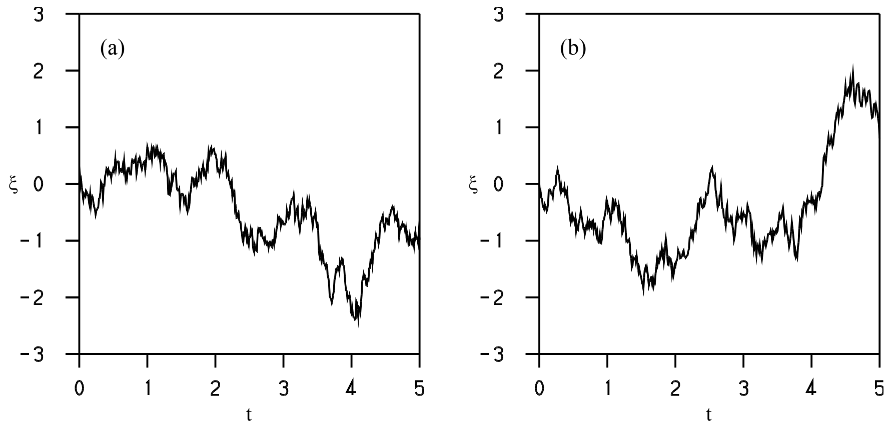

Fig. 3.2. Two examples for realizations of the stochastic equation (3.48).

coefficients vanish because they are of higher order in Δt. Hence, the stochastic equation (3.42) uniquely determines a Fokker-Planck equation that describes the PDF evolution. However, the opposite is not the case in general. For N variables, equation (3.47b) represents N (N + 1) / 2 equations for N^2 elements of b_{ij}. Thus, the coefficients of the equation (3.42) are uniquely determined by the coefficients D_i and D_{ij} of the Fokker-Planck equation only if b_{ij} is assumed to be symmetric.

3.4.3. Monte Carlo simulation

Applications of Fokker-Planck equations to turbulent reacting flows often require the consideration of a large number of variables, which makes the direct solution of Fokker-Planck equations extremely complicated or even impossible. This problem can be avoided if stochastic differential equations are used which correspond to a given Fokker-Planck equation. This means one solves equation (3.42) with a_i and (a symmetric) b_{ij}, which are derived according to the relations (3.47a-b) from the coefficients D_i and D_{ij} of a Fokker-Planck equation.

The advantage of such Monte Carlo simulations is given by the fact that stochastic equations can be solved easily. The statistics of ΔW_k, which are required to solve (3.44), are available in standard routines, and all the means and the PDF of a stochastic process considered can be obtained by summation. Suitable techniques to solve such equations are described, e.g., by Kloeden and Platen (1992). As an example, two realizations of a specification of (3.42)

$$\frac{d\xi}{dt} = -\xi + \frac{dW}{dt}, \tag{3.48}$$

are shown in Fig. 3.2. These solutions were obtained for $\xi(0) = 0$ and $\Delta t = 0.01$.

The drawback of Monte Carlo methods for the solution of Fokker-Planck equations is that they are often time-consuming, and generally have high memory requirements. The statistical accuracy decreases only with $N^{1/2}$, where N is the number of realizations (Risken 1984). Hence, one needs, for example, 100 times more particles to improve the accuracy by an order of magnitude. Correspondingly, the deviations from the exact mean and variance of $\Delta W_k / (\Delta t)^{1/2}$ are about 1% if 10^4 realizations are considered, and 0.1% for 10^6 realizations.

3.5. Stochastic modeling

The reduction of the general stochastic model (3.41) to the Markov model (3.42) is a very important step regarding the construction of a stochastic model for any specific case considered. However, to obtain closed stochastic differential equations one still has to solve two important problems: one has to choose an appropriate set of stochastic variables, and the coefficients in the stochastic equations have to be determined as functions of the variables considered.

3.5.1. The set of variables considered

The first problem to find a suitable set of stochastic variables can be solved by estimating the correlation time scale of the forces that drive the dynamics of the quantities of interest. Usually, one will find that this time scale is nonzero, such that the structure of equation (3.42) cannot be used directly. However, as pointed out in detail in Appendix 3A, it is then possible to extend the set of variables considered such that (3.42) can be used. A detailed application of this concept will be given in chapter 5 regarding the construction of models for turbulent velocities.

3.5.2. The coefficients of stochastic equations

The second problem to provide the coefficients a_i and b_{ik} in the stochastic equation (3.42) as explicit functions of the stochastic variables can be addressed in the following way. In many cases one can find simple and well-justified parametrizations for the diffusion coefficient b_{ik}. This is not surprising because b_{ik} just simulates the intensity of the unordered, chaotic production of fluctuations. The determination of a_i is much more complicated. Simple solutions (isotropic linear relaxation models) are available for systems in equilibrium states, and the extension of such equations (anisotropic linear relaxation models with mixing frequencies that vary in space and time) for the simulation of systems in near-equilibrium states does often work successfully. However, the simulation of nonequilibrium processes requires the consideration of nonlinear stochastic models. Various ways to construct them will be discussed in chapter 5.

Appendix 3A: The dynamics of relevant variables

A systematic procedure for the construction of stochastic equations for any variables considered (which will be referred to as relevant variables) will be presented here. This methodology is called the projection operator technique. Its basic idea is to extract the dynamics of relevant variables from any complete, deterministic dynamics. This results in contributions to the dynamics of relevant variables that are explicit deterministic functions of the relevant variables (which may involve memory effects), and remaining contributions that involve the influence of all the other quantities. The latter terms have the properties of stochastic forces.

The projection operator technique may be applied in various variants, see for instance Grabert (1982), Lindenberg & West (1990) and Zubarev et al. (1996, 1997). One way is to derive a PDF transport equation for relevant variables, which has (by adopting the Markov assumption) a structure that corresponds to that of the Fokker-Planck equation. Another way is to separate the instantaneous dynamics of relevant variables from the complete dynamics, see Heinz (1997). This approach will be presented here to contrast the derivation of PDF transport equations in the sections 3.1 and 3.2 with a corresponding construction of stochastic models.

3A.1. The problem considered

We assume that the dynamics of a system considered are completely described by a set of variables $\boldsymbol{\Xi}(t) = \{\boldsymbol{\xi}(t), \boldsymbol{\eta}(t)\}$, see Fig. 2.1 in chapter 2 for an illustration. The vector $\boldsymbol{\xi}(t)$ refers to variables that we consider to be relevant, and $\boldsymbol{\eta}(t)$ denotes the vector of the remaining (irrelevant) variables. Instead of $\boldsymbol{\Xi}(t)$, we may consider the corresponding instantaneous PDF $\Psi^*(\mathbf{x}, \mathbf{y}, t) = \delta(\boldsymbol{\xi}(t) - \mathbf{x})\, \delta(\boldsymbol{\eta}(t) - \mathbf{y})$. An equation for the evolution of this PDF may be obtained by differentiating it by time. This results in

$$\frac{\partial \Psi^*(\mathbf{x}, \mathbf{y}, t)}{\partial t} = -\left[\frac{\partial}{\partial x_k} \frac{d\xi_k}{dt}(\boldsymbol{\xi}(t), \boldsymbol{\eta}(t), t) + \frac{\partial}{\partial y_n} \frac{d\eta_n}{dt}(\boldsymbol{\xi}(t), \boldsymbol{\eta}(t), t)\right] \Psi^*(\mathbf{x}, \mathbf{y}, t). \quad (3A.1)$$

The derivatives by the arguments of the delta functions are rewritten into the corresponding sample space derivatives ($\partial \Psi^* / \partial(\xi_1(t) - x_1) = - \partial \Psi^* / \partial x_1$). The sample space derivatives may be drawn in front of $d\xi_k / dt$ and $d\eta_n / dt$ since the latter are independent of $\mathbf{x}$ and $\mathbf{y}$. Equation (3A.1) corresponds to the Liouville equation of classical statistical mechanics. It is unclosed due to the appearance of the unknown derivatives $d\xi_k / dt$ and $d\eta_n / dt$. The explicit time dependence in these derivatives may be caused for instance by the appearance of external forces.

In general, there is neither a way to assess the detailed dynamics of the complete set of variables $\mathbf{\Xi}(t)$ nor an interest to have all this information. Therefore, we restrict the attention to the dynamics of relevant variables $\boldsymbol{\xi}(t)$, which may by obtained from (3A.1) by integration over the **y**-space. This leads to

$$\frac{\partial\Psi(\mathbf{x},t)}{\partial t}=-\frac{\partial}{\partial x_k}\frac{d\xi_k}{dt}(\xi(t),\boldsymbol{\eta}(t),t)\Psi(\mathbf{x},t)=\left[L^{rel}(\mathbf{x},t)+L^{ext}(\mathbf{x},t)+L(\mathbf{x},\boldsymbol{\eta},t)\right]\Psi(\mathbf{x},t), \tag{3A.2}$$

where the instantaneous PDF of the process $\boldsymbol{\xi}(t)$ is referred to

$$\Psi(\mathbf{x},t)=\delta(\xi(t)-\mathbf{x}). \tag{3A.3}$$

The sum of the operators L^{rel}, L^{ext} and L is defined by the middle expression of (3A.2). This differentiation of different contributions to the evolution of relevant variables is applied to refer to the possibility of the appearance of contributions that are explicit functionals of the relevant variables, this means contributions that do not require assumptions to take them into account. Terms related to L^{rel} are found, e.g., if x_n denotes coordinates in physical space and $d\xi_n$ / dt corresponding velocities. L^{ext} refers to a possible contribution due to external forces, which is also assumed to be known. Due to the fact that the consideration of L^{rel} and L^{ext} does not pose any difficulties, we will neglect them for simplicity. Consequently, we consider the following basic equation

$$\frac{\partial}{\partial t}\Psi(\mathbf{x},t)=L(\mathbf{x},\boldsymbol{\eta},t)\Psi(\mathbf{x},t). \tag{3A.4}$$

Regarding the dynamics of $\xi(t)$, equation (3A.4) is unclosed due to the appearance of irrelevant variables $\boldsymbol{\eta}(t)$. The rewriting of (3A.4) by means of the projection operator technique will be considered next.

3A.2. The projection operator

To rewrite the dynamics (3A.4) we need a projection operator P that projects any functions A = A($\boldsymbol{\xi}$(t), $\boldsymbol{\eta}$(t), t) of relevant and irrelevant variables onto the subspace of relevant variables. Such an operator will be defined by

$$PA(\xi(t),\boldsymbol{\eta}(t),t)=\int d\mathbf{x}\,\left\langle A(\xi(t),\boldsymbol{\eta}(t),t)\,\middle|\,\xi(0)=\mathbf{x}\right\rangle\Psi(\mathbf{x},0), \tag{3A.5}$$

where the initial time is assumed to be zero. The conditional mean on the right-hand side is defined by (2.35). P is characterized by the properties (A and B are any functions of relevant and irrelevant variables)

$$\langle(PA)\,B\rangle=\langle A\,(PB)\rangle, \qquad P\,\Psi(\mathbf{x},0)=\Psi(\mathbf{x},0), \qquad P^2=P. \tag{3A.6}$$

The validity of the relations (3A.6) may be proved by means of (3A.5) combined with the definition (2.35) of conditional means,

$$\langle (PA)B \rangle = \int d\mathbf{x} \langle A \,|\, \xi(0) = \mathbf{x} \rangle \langle \Psi(\mathbf{x},0) B \rangle = \int d\mathbf{x} \langle B \,|\, \xi(0) = \mathbf{x} \rangle \langle A\, \Psi(\mathbf{x},0) \rangle = \langle A (PB) \rangle,$$

$$P\Psi(\hat{\mathbf{x}},0) = \int d\mathbf{x} \langle \Psi(\hat{\mathbf{x}},0) | \xi(0) = \mathbf{x} \rangle \Psi(\mathbf{x},0) = \int d\mathbf{x}\, \delta(\mathbf{x} - \hat{\mathbf{x}}) \Psi(\mathbf{x},0) = \Psi(\hat{\mathbf{x}},0),$$

$$P^2 A = \int d\hat{\mathbf{x}} \left\langle \int d\mathbf{x} \langle A \,|\, \xi(0) = \mathbf{x} \rangle \Psi(\mathbf{x},0) \middle| \xi(0) = \hat{\mathbf{x}} \right\rangle \Psi(\hat{\mathbf{x}},0)$$

$$= \int d\hat{\mathbf{x}} \langle A \,|\, \xi(0) = \hat{\mathbf{x}} \rangle \Psi(\hat{\mathbf{x}},0) \left\langle \int d\mathbf{x}\, \Psi(\mathbf{x},0) \middle| \xi(0) = \hat{\mathbf{x}} \right\rangle = PA. \tag{3A.7}$$

Alternatively, the relations (3A.6) may be formulated by adopting the complement operator Q = 1 − P,

$$\langle (QA)\, B \rangle = \langle A\, (QB) \rangle, \qquad Q\Psi(\mathbf{x},0) = 0, \qquad Q^2 = Q. \tag{3A.8}$$

The latter relations will be used frequently below.

3A.3. An operator identity

To transform (3A.4) in the way described above we consider its formal solution

$$\Psi(\mathbf{x},t) = e^{Lt}\Psi(\mathbf{x},0) = \left\{ 1 + \sum_{n=1}^{\infty} \frac{t^n}{n!} L^n \right\} \Psi(\mathbf{x},0). \tag{3A.9}$$

The operator exp(Lt) can be considered as the sum of two contributions,

$$e^{Lt} = U_1(t) + U_2(t), \tag{3A.10}$$

where U_1 describes the part of the dynamics which is explicit in the relevant variables (it may depend on all the history of the relevant variables), and U_2 is the remainder, i.e., U_2 a function of the irrelevant variables. To determine U_2, we will assume that it is determined by the following equation and initial condition,

$$\frac{dU_2}{dt} = QLU_2, \qquad U_2(0) = 1. \tag{3A.11}$$

Due to PQ = P (1 − P) = 0, which follows from the last part of (3A.6), the assumed evolution equation for U_2 assures that the projection of dU_2 / dt vanishes in the ensemble average. This enables the interpretation of dU_2 / dt as a stochastic force, see the explanations given below. The condition $U_2(0) = 1$ implies $U_1(0) = 0$. This corresponds with the assumption that $U_1(t)$ is independent of its initial condition. As a consequence of (3A.11), U_1 is determined by the following equation and initial condition,

$$\frac{dU_1}{dt} = \frac{de^{Lt}}{dt} - \frac{dU_2}{dt} = LU_1 + PLU_2, \qquad U_1(0) = 0. \tag{3A.12}$$

By adopting the formal solutions of (3A.11) and (3A.12), the evolution operator exp(Lt) can be rewritten into

$$e^{Lt} = e^{QLt} + \int_0^t dt'\, e^{L(t-t')} PLe^{QLt'}. \tag{3A.13}$$

We transform the integrand by setting t' = t − s. This results in the operator identity

$$e^{Lt} = e^{QLt} + \int_0^t ds\, e^{Ls} PLe^{QL(t-s)}. \tag{3A.14}$$

Its consistency may be seen by comparing the initial values and derivatives by t of both sides.

3A.4. The dynamics of relevant variables

The use of the operator identity (3A.14) in (3A.9) allows now the rewriting of the evolution equation (3A.4). By adopting the definition (3A.5) of the projection operator P we obtain

$$\Psi(\hat{\mathbf{x}}, t) = \int_0^t ds \int d\mathbf{x} \left\langle Le^{QL(t-s)} \Psi(\hat{\mathbf{x}}, 0) \middle| \boldsymbol{\xi}(0) = \mathbf{x} \right\rangle \Psi(\mathbf{x}, s) + e^{QLt}\, \Psi(\hat{\mathbf{x}}, 0). \tag{3A.15}$$

We differentiate (3A.15) by time, multiply it by x_i and integrate it over the space of relevant variables. This leads to the following equation for relevant variables ξ_i,

$$\frac{d\xi_i}{dt} = -\int d\mathbf{x}\, M_i(\mathbf{x}, 0)\, \Psi(\mathbf{x}, t) - \int_0^t ds \int d\mathbf{x}\, \frac{dM_i}{dt}(\mathbf{x}, t-s)\, \Psi(\mathbf{x}, s) + f_i(t), \tag{3A.16}$$

where we applied the abbreviations

$$M_i(\mathbf{x}, t) = -\int d\hat{\mathbf{x}}\; \hat{x}_i \left\langle Le^{QLt} \Psi(\hat{\mathbf{x}}, 0) \middle| \boldsymbol{\xi}(0) = \mathbf{x} \right\rangle, \tag{3A.17a}$$

$$f_i(t) = \int d\hat{\mathbf{x}}\; \hat{x}_i QLe^{QLt} \Psi(\hat{\mathbf{x}}, 0) = QLe^{QLt} \xi_i(0). \tag{3A.17b}$$

The last term f_i in equation (3A.16) is a function of the irrelevant variables. By adopting the relations (3A.8), we find

$$\langle f_i(t)\, \Psi(\mathbf{x}, 0) \rangle = \langle Qf_i(t)\, \Psi(\mathbf{x}, 0) \rangle = \langle f_i(t)\, Q\Psi(\mathbf{x}, 0) \rangle = 0. \tag{3A.18}$$

The integration of this relation over **x** leads then to the result

$$\langle f_i(t) \rangle = 0. \tag{3A.19}$$

This important property of f_i to vanish in the ensemble mean enables its interpretation as a stochastic force.

The first two terms on the right-hand side of equation (3A.16) are functions of relevant variables. They are characterized by the memory function $M_i(\mathbf{x}, t)$, which represents the averaged influence of irrelevant variables on the dynamics of relevant variables. By means of (3.17a), we find for $M_i(\mathbf{x}, 0)$, which appears in the first term,

$$M_i(\mathbf{x},0) = -\left\langle \frac{d\xi_i}{dt}(0) \middle| \boldsymbol{\xi}(0) = \mathbf{x} \right\rangle. \tag{3A.20}$$

This expression may be rewritten into an equation that relates $M_i(\mathbf{x}, 0)$ to the PDF $<\delta(\boldsymbol{\xi}(t) - \mathbf{x})>$,

$$\frac{\partial}{\partial x_i} M_i(\mathbf{x},0) \langle \Psi(\mathbf{x},0) \rangle = -\frac{\partial}{\partial x_i} \left\langle \Psi(\mathbf{x},0) \frac{d\xi_i}{dt}(0) \right\rangle = \left[\frac{\partial}{\partial t} \langle \Psi(\mathbf{x},t) \rangle \right] (t=0). \tag{3A.21}$$

This result shows that $M_i(\mathbf{x}, 0)$ vanishes under stationary conditions. With regard to $dM_i(\mathbf{x}, t) / dt$ in the second term on the right-hand side of (3A.16) we obtain by the differentiation of the expression (3A.17a)

$$\frac{dM_i}{dt}(\mathbf{x},t) = -\langle L f_i(t) \,|\, \boldsymbol{\xi}(0) = \mathbf{x} \rangle. \tag{3A.22}$$

This relation is an essential result of the approach presented here. It provides a link between the stochastic force f_i, which generates fluctuations of relevant variables, and $dM_i(\mathbf{x}, t) / dt$, which controls the relaxation (the dissipation) of fluctuations of relevant variables. Such relations are called fluctuation-dissipation theorems. The value of (3A.22) arises from the possibility of calculating the function $dM_i(\mathbf{x}, t) / dt$ on the basis of assumption about the statistics of stochastic forces. This will be pointed out in the next three subsections.

3A.5. The equilibrium dynamics of relevant variables

The use of the fluctuation-dissipation theorem (3A.22) for the calculation of $dM_i(\mathbf{x}, t) / dt$ requires assumptions on L to relate the right-hand side to measurable quantities. For statistically stationary processes, L is characterized by the property

$$\frac{\partial \langle AB \rangle}{\partial t} = 0 = \langle (LA)B \rangle + \langle A(LB) \rangle. \tag{3A.23}$$

This relation may be used to rewrite the expression (3A.22). We obtain

$$\frac{dM_i}{dt}(\mathbf{x},t)\left\langle\Psi(\mathbf{x},0)\right\rangle = -\left\langle Lf_i(t)\,\Psi(\mathbf{x},0)\right\rangle = \left\langle f_i(t)\,L\Psi(\mathbf{x},0)\right\rangle = \left\langle f_i(t)\,QL\Psi(\mathbf{x},0)\right\rangle$$

$$= -\frac{\partial}{\partial x_k}\left\langle f_i(t)\,\Psi(\mathbf{x},0)\,QL\xi_k(0)\right\rangle = -\frac{\partial}{\partial x_k}\left\langle f_i(t)\,f_k(0)\,\Psi(\mathbf{x},0)\right\rangle$$

$$= -\frac{\partial}{\partial x_k}\left\langle f_i(t)\,f_k(0)\,\middle|\,\boldsymbol{\xi}(0)=\mathbf{x}\right\rangle\left\langle\Psi(\mathbf{x},0)\right\rangle. \qquad (3A.24)$$

The first rewriting of the left-hand side results from the definition (2.35) of conditional means. The second rewriting makes use of (3A.23). Then, we replace f_i by Q f_i, and apply the first part of relation (3A.8) to obtain the third rewriting. The expressions on the second line may be obtained by applying L to $\Psi(\mathbf{x}, 0)$ and adopting the definition (3A.17b) of stochastic forces. The definition of conditional means is then applied again to obtain the last line of (3A.24).

The application of the relation (3A.24) in equation (3A.16) implies then the following equilibrium dynamics of relevant variables,

$$\frac{d\xi_i}{dt} = \int_0^t ds \int d\mathbf{x}\, \left\langle\Psi(\mathbf{x},0)\right\rangle^{-1} \frac{\partial\left\langle f_i(t-s)\,f_k(0)\,\middle|\,\boldsymbol{\xi}(0)=\mathbf{x}\right\rangle\left\langle\Psi(\mathbf{x},0)\right\rangle}{\partial x_k}\,\Psi(\mathbf{x},s) + f_i(t),$$

$$(3A.25)$$

where $M_i(\mathbf{x}, 0) = 0$ is applied for the stationary case considered. Thus, the specification of the equilibrium PDF $<\Psi(\mathbf{x}, 0)>$ and statistics of the stochastic force f_i completely determines the dynamics of relevant variables. Examples for such assumptions will be considered next.

3A.6. Colored Gaussian noise

The consideration of the vector of relevant variables $\boldsymbol{\xi}(t)$ as a continuous process requires the assumption that the stochastic force f_i is a Gaussian process (Gardiner 1983, Thomson 1987). Therefore, f_i is completely specified by its zero mean and correlation. First, we will assume that f_i is a colored noise process, this means its correlation function is characterized by an exponential function,

$$\left\langle f_i(t)f_k(s)\right\rangle = \left\langle f_i(t-s)f_k(0)\right\rangle = \frac{1}{2\tau_f} b_{in} b_{kn} \exp\left\{-\frac{|t-s|}{\tau_f}\right\}. \qquad (3A.26)$$

b_{in} denotes a constant coefficient and τ_f represents the constant correlation time of f_i. The first rewriting of the left-hand side results from the fact that the correlation function only depends on the difference of the time argument under statistically stationary conditions. The use of (3A.26) in equation (3A.25) leads then to the equilibrium dynamics

$$\frac{d\xi_i}{dt} = -\frac{1}{2\tau_f} b_{in} b_{kn} \sigma^{-1}{}_{km} \int_0^t ds \, \exp\left\{-\frac{t-s}{\tau_f}\right\} \left(\xi_m(s) - \langle \xi_m \rangle\right) + f_i(t) \tag{3A.27}$$

if the equilibrium PDF is specified as a Gaussian PDF with constant variance matrix σ. The inverse variance matrix is denoted by σ^{-1}.

The inclusion of correlated noise and memory effects in (3A.27) hampers analyses and the application of standard methods for the solution of stochastic differential equations (Kloeden & Platen 1992). In order to rewrite equation (3A.27), we represent f_i as solution of the equation

$$\frac{df_i}{dt} = -\frac{1}{\tau_f} f_i + \frac{1}{\tau_f} b_{in} \frac{dW_n}{dt}. \tag{3A.28}$$

By adopting the relations between stochastic equations and Fokker-Planck equations pointed out in section 3.4 in combination with the findings presented in section 3.3, one can prove that this equation determines f_i as a Gaussian process. Its means vanish for the assumed stationarity, and the correlation function of f_i satisfies for $s \geq 0$ according to (3.40) the equation

$$\frac{\partial}{\partial s} \langle f_i(t) f_k(t+s) \rangle = -\frac{1}{\tau_f} \langle f_i(t) f_k(t+s) \rangle. \tag{3A.29}$$

This equation provides the same evolution of the correlation function of f_i as given by (3A.26). Therefore, the definition of f_i by (3A.28) is equivalent to (3A.26) provided the variance of f_i (which represents the initial condition to equation (3A.29)) is also consistent with the corresponding implication of (3A.26),

$$\langle f_i(t) \, f_k(t) \rangle = \frac{1}{2\tau_f} b_{in} b_{kn}. \tag{3A.30}$$

This is the case, see equation (3.36b) for the stationary case considered.

By adopting (3.A28) we can transform (3A.27) into the frame of the stochastic equations (3.42). This may be seen by differentiation of (3A.27),

$$\begin{aligned} \frac{d}{dt}\frac{d\xi_i}{dt} &= -\frac{1}{2\tau_f} b_{in} b_{kn} \sigma^{-1}{}_{km} \left(\xi_m(t) - \langle \xi_m \rangle\right) - \frac{1}{\tau_f}\left(\frac{d\xi_i}{dt} - f_i(t)\right) + \frac{df_i}{dt} \\ &= -\frac{1}{2\tau_f} b_{in} b_{kn} \sigma^{-1}{}_{km} \left(\xi_m(t) - \langle \xi_m \rangle\right) - \frac{1}{\tau_f}\frac{d\xi_i}{dt} + \frac{1}{\tau_f} b_{in} \frac{dW_n}{dt}. \end{aligned} \tag{3A.31}$$

Hence, the enlarged set of variables (ξ, $d\xi$ / dt) represents a Markov process that satisfies the structure of the equations (3.42). Such a rewriting of the equations (3A.27) is usually very helpful because many results related to Fokker-Planck equations and their solutions can be applied then.

3A.7. White Gaussian noise

A further specification of the dynamics of relevant variables is given by the assumption that f_i becomes delta-correlated ($\tau_f \to 0$). In this case, the correlation function (3A.26) reduces to

$$\langle f_i(t)\, f_k(s)\rangle = \lim_{\tau_f \to 0} \frac{1}{2\tau_f} b_{in} b_{kn} \exp\left\{-\frac{|t-s|}{\tau_f}\right\}\delta_{ik} = b_{in} b_{kn} \delta(t-s). \qquad (3A.32)$$

The comparison of the properties of f_i with those of dW_i / dt, see the relations (3.43a-b), shows that f_i has to be proportional to dW_i / dt in this case. This relation can be derived from the stochastic model (3A.28) for f_i, which reduces for $\tau_f \to 0$ to the expression

$$f_i(t) = b_{ik} \frac{dW_k}{dt}. \qquad (3A.33)$$

The use of (3A.32) and (3A.33) in (3A.27) leads then to the equation

$$\frac{d\xi_i}{dt} = -\frac{1}{2} b_{in} b_{nk} \sigma^{-1}{}_{km}\left(\xi_m - \langle \xi_m \rangle\right) + b_{in} \frac{dW_n}{dt}. \qquad (3A.34)$$

Thus, for the case of white-noise forces f_i one obtains equations for the set $\xi(t)$ of relevant variables which agree with the structure of the stochastic equations (3.42).