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STOCHASTIC PROCESSES: TIME EVOLUTION, SYMMETRIES AND LINEAR RESPONSE

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Abstract:

We give a systematic survey of the theory of stochastic processes in systems described by a finite number of variables, with special emphasis on time evolution behaviour, symmetry aspects, and linear response to external perturbations. The concepts and methods are elucidated by the application to a number of specific systems.

Introduction

The theory of stochastic processes plays an important role in the description of systems which do not behave in a deterministic way, but display statistical fluctuations of the system variables. Such systems occur in many fields of science, in particular in physics and the applied sciences, in communication theory, in biology and environmental sciences, and even in sociology [1–18].

Statistical fluctuations in classical systems always reflect a lack of knowledge about the exact state of the system. A large system is described in terms of a few macrovariables obtained by "coarse-graining" in phase space, and the loss of knowledge about the microscopic degrees of freedom gives rise to "intrinsic" fluctuations of the microvariables [3, 6, 14]. Further, the external forces in the equations of motion, which describe the coupling of the system to the outside, have also to be considered as fluctuating quantities, because they are produced by other macroscopic systems. They impose "external" fluctuations on the system under consideration. The distinction between intrinsic and external fluctuations will of course depend on where the boundary is drawn between "system" and "outside". Quantum fluctuations, on the contrary, occur even in a pure state.

On a microscopic scale, fluctuations play a dominant role in statistical mechanics. Fluctuations of the macroscopic variables, on the other hand, are usually very small, but have nevertheless important effects in certain situations. We mention in particular the scattering of light or of particles by the system, the occurrence of critical fluctuations near phase transitions and instabilities, and the decay of metastable states [1, 5, 7–18].

We present here a review of the theory of classical stochastic processes, with strong emphasis on pedagogic aspects. The theory is applicable to classical systems, and to such quantum systems which allow an appropriate semiclassical description. In section 1, we give a survey of the basic concepts and properties of stochastic processes, described in terms of the multiple-time joint probability distribution functions. We introduce the important class of Markov processes for which the whole hierarchy of multiple-time distribution functions is generated by the two-time conditional probability distribution. This represents an enormous simplification, and most of the present review will be restricted to the Markov class. The justification for this restriction rests on the separation of the time scales of microscopic and macroscopic motion: If all slow variables of the system are included among the macroscopic variables, the Markov description of the process is expected to be justified for macroscopic times.

The time evolution of stochastic processes is discussed in section 2. For a Markov process, the time derivative of the conditional probability has the significance of a "master operator" generating the time evolution of the whole process. It is of as fundamental importance for a Markov process as the

Hamiltonian for deterministic motion, and is therefore the object of stochastic modelling: Constructing a stochastic model for a given system is in the Markov case equivalent to constructing a master operator. We discuss in some detail the master operators of jump processes and of continuous stochastic processes (Fokker–Planck processes), and in particular the description of the latter by stochastic differential equations.

In section 3, we review the spectral properties of a stochastic process. The spectrum of the master operator completely governs the dynamics of a Markov process, yielding in particular the properties of the correlation functions in the time and frequency domains. The asymptotic behaviour for long times depends crucially on the ergodic properties of the process, which are therefore also discussed in this section.

Section 4 is devoted to a discussion of symmetry aspects. Due to the inherent nonlinearities in the macroscopic motion, it is in general not a trivial problem to obtain solutions of the master equation. Symmetry considerations often provide essential information about the form and the properties of the solution, and may even allow to construct the solution explicitly. In particular, the symmetry of detailed balance involving an interchange of time arguments in the stationary multiple-time joint probability distribution has proved to be very effective [3, 5, 8, 11].

The concept of linear response to external test forces has proved very useful for the study of systems in thermal equilibrium as well as of driven systems. It yields valuable information about the dynamics of the system, expecially about the stability and the normal modes. Of particular importance is the fluctuation-dissipation theorem of equilibrium systems [7]. We therefore develop in section 5 the linear-response theory for Markov processes, with special attention towards the existence of fluctuation theorems connecting the linear response to external perturbations with the unperturbed fluctuations of the system.

Throughout the review, we demonstrate the application of the concepts and the methods by specific examples in the subsections denoted by the letter E. In particular, the various subsections concerning the two-state process and the n-component Gauss process comprise in themselves a fairly detailed and selfcontained compilation of the properties of these two types of stochastic processes.

In section 6, we apply the theory presented in this survey to a number of physical systems: The Brownian motion in an external potential, the nonlinear conductance, the bistable tunnel diode, the single-mode laser, and the stochastic Ising model with a number of specific applications. These problems, in addition to serving as demonstration objects for the general theory, are of considerable interest in their own right.

1. Basic concepts

In order to make this report self-contained, we give a brief survey of the basic concepts of stochastic processes.

1.1. Probability distributions, random variables, fluctuations

The stochastic systems considered may be of the following types:
Type A: Systems with a finite or countable number of discrete states $\alpha = 1, 2, \ldots,$
Type B: Systems described by a finite number of real or complex continuous state variables x_i forming the *state vector*

$$\boldsymbol{x} = \{x_1, x_2, \ldots\},$$

Type C: Systems described by a finite number of stochastic fields

$$\phi_i(\boldsymbol{r}),\ i = 1, 2, \ldots N.$$

Examples for systems of type A are the stochastic Ising model [19] (see section 6.5) and various systems described by birth and death processes [20–22] (see e.g. section 6.3). As systems of type B we mention the Brownian particle described by position and momentum (see section 6.1), and the laser described by a finite number of mode amplitudes [1, 2, 5, 8, 11, 16] (see section 6.4 for the single-mode laser). If the space dependence of some variables becomes important, as e.g. in hydrodynamics, one deals with a system of type C.

The set of all states of the system is called the *state space* Σ. A stochastic state of the system is given by a probability distribution on Σ. For the three cases introduced above it is described in the following way:

Type A: The stochastic state is described in terms of the probabilities p_α of the states α satisfying

$$0 \leq p_\alpha \leq 1, \qquad \alpha = 1, 2, \ldots N \tag{1.1.1}$$

$$\sum_{\alpha \in \Sigma} p_\alpha = 1. \tag{1.1.2}$$

The probability of any subset $A \subseteq \Sigma$ is given by

$$p(A) = \sum_{\alpha \in A} p_\alpha. \tag{1.1.3}$$

Type B: We assume the existence of a probability density $p(\boldsymbol{x})$ in state space Σ satisfying

$$p(\boldsymbol{x}) \geq 0 \qquad \forall x \in \Sigma \tag{1.1.4}$$

$$\int_{\Sigma} p(\boldsymbol{x})\, \mathrm{d}x = 1. \tag{1.1.5}$$

$p(\boldsymbol{x})$, which may contain δ-functions and is therefore a distribution in the mathematical sense, well be called the *probability distribution* describing the stochastic state of the system. The probability of any measurable subset $A \subseteq \Sigma$ is given by

$$p(A) = \int_{A} p(\boldsymbol{x})\, \mathrm{d}x. \tag{1.1.6}$$

In the case of complex state variables, the integral is defined over the complex planes: $\mathrm{d}x = \prod \mathrm{dRe}x_i\ \mathrm{dIm}x_i$.

Type C: In this case, the stochastic state is described by a probability distribution in function space,

which requires the methods of functional integration, and will not be treated in detail. A short discussion is given in section 2.5. In the case of systems enclosed in a finite boundary, the fields can be decomposed into countable sets of discrete modes, the amplitudes of which form a state space which is a slightly extended version of type B.

The general theory is developed for type B. Specialization to type A will always be evident. Generalization to type C will be indicated in special cases.

The set of all probability distributions with $p(\Sigma) = 1$ forms a functional manifold $\Pi^*(\Sigma)$ (not a linear space). In order to define linear operators, it is useful to complete this manifold to a linear function space $\Pi(\Sigma)$. Throughout this review, we shall use the following notation: State functions $f \in \Pi(\Sigma)$ and distributions $p \in \Pi^*(\Sigma)$ are denoted by their function names f, p, their values at point $x \in \Sigma$ by $f(x)$, $p(x)$. Operators acting on $\Pi(\Sigma)$ are described by their kernels $A \in \Pi(\Sigma \otimes \Sigma)$ with values $A(x, y)$. Application of an operator A to an element $f \in \Pi(\Sigma)$, and successive action of two operators A, B are written in the usual way as products Af and BA, respectively,

$$(Af)_x = \int A(x, y) f(y)\, dy \tag{1.1.7}$$

$$(BA)_{x,y} = \int B(x, z) A(z, y)\, dz\,. \tag{1.1.8}$$

All integrations are over the full state space Σ unless otherwise indicated.

A basic concept is that of a *random variable* f corresponding to an observable quantity. It may be any real or complex measurable state function $f \in \Pi(\Sigma)$

$$f\colon \Sigma \to \mathbb{R} \text{ or } \mathbb{C}\,, \tag{1.1.9}$$

in particular any of the state variables x_i themselves.

A mapping

$$q\colon \Sigma^{(x)} \to \Sigma^{(q)} \tag{1.1.10}$$

of the original state space $\Sigma^{(x)}$ onto the space $\Sigma^{(q)}$ spanned by the set $q = \{q_1, q_2, \ldots\}$ of random variables may be considered as the introduction of a new state space $\Sigma^{(q)}$ with state vectors q. The probability distribution in $\Sigma^{(q)}$ is given by

$$p(q) = \int \delta(q(x) - q)\, p(x)\, dx\,. \tag{1.1.11}$$

If the mapping (1.1.10) is one-to-one, it is equivalent to a coordinate transformation in the original state space. If it is many-to-one, on the other hand, it represents a *coarse-graining* of state space. In the following we assume that the state variables $x = \{x_1, x_2, \ldots\}$ characterize the states of the system at the desired level of description, i.e. that the appropriate coarse-graining has already been carried out.

Two random variables f and g are *statistically independent* if

$$p(f, g) = p(f)\, p(g)\,. \tag{1.1.12}$$

The *statistical expectation value* or *mean value* of the random variable f is given by

$$\langle f \rangle = \int f(x)\, p(x)\, \mathrm{d}x\,, \tag{1.1.13}$$

and the *equal-time correlation* between two random variables f and g is defined as

$$\langle f g^* \rangle = \int f(x)\, g^*(x)\, p(x)\, \mathrm{d}x\,. \tag{1.1.14}$$

The *fluctuation* of the random variable f is the state function

$$\varphi = f - \langle f \rangle \tag{1.1.15}$$

with $\langle \varphi \rangle = 0$. A measure for the fluctuation strength is the *mean-square fluctuation* or *variance*

$$\langle |\varphi|^2 \rangle = \langle |f|^2 \rangle - |\langle f \rangle|^2\,. \tag{1.1.16}$$

The fluctuations $\varphi = f - \langle f \rangle$ of a set of random variables $f = \{f_1, f_2, \ldots\}$ can be characterized by the non-negative definite equal-time *covariance matrix*

$$\mathbf{S} = \langle \varphi \varphi^* \rangle = \langle f f^* \rangle - \langle f \rangle \langle f^* \rangle\,, \tag{1.1.17}$$

which contains the variances $\langle |\varphi_i|^2 \rangle$ as diagonal elements and the correlations between the fluctuations $\langle \varphi_i \varphi_j^* \rangle$ as nondiagonal elements. Since $\mathbf{S}$ is Hermitian, there exists a unitary transformation to uncorrelated linear combinations of the f_i. It should be noted that uncorrelated random variables f_i with $\langle f_i f_j^* \rangle = \langle |f_i|^2 \rangle \delta_{ij}$ are in general not statistically independent.

For a detailed review of the main concepts of random variables, especially cumulants, characteristic functions, etc. see [23, 24].

1.1.E1. The two-state distribution

A simple example of a system of type A is a two-state system with an Ising variable $x_\alpha = \pm 1$. It is described by a probability distribution

$$p \triangleq \frac{1}{2}\begin{pmatrix} 1+a \\ 1-a \end{pmatrix} = \frac{1}{2}(1+ax)\,, \qquad |a| \leqslant 1\,, \tag{1.1.18}$$

and is completely characterized by the mean value,

$$\langle x \rangle = \sum x_\alpha p_\alpha = a\,. \tag{1.1.19}$$

The mean square of the fluctuation $\xi = x - \langle x \rangle$ is given by

$$\langle \xi^2 \rangle \equiv s = 1 - a^2 \geq 0\,. \tag{1.1.20}$$

1.1.E2. The n-component Gaussian distribution

As an example of type B we consider a Gaussian distribution of a set $\boldsymbol{x} = (x_1, x_2, \ldots x_n)$ of n real random variables,

$$p(\boldsymbol{x}) = [\det(2\pi \mathbf{s})]^{-1/2} \exp[-\tfrac{1}{2}(\boldsymbol{x} - \boldsymbol{a}) \cdot \mathbf{s}^{-1} \cdot (\boldsymbol{x} - \boldsymbol{a})] \,. \tag{1.1.21}$$

It is completely characterized by the vector of mean values

$$\langle \boldsymbol{x} \rangle = \boldsymbol{a} \tag{1.1.22}$$

and the covariance matrix of the fluctuations $\boldsymbol{\xi} = \boldsymbol{x} - \langle \boldsymbol{x} \rangle$,

$$\langle \boldsymbol{\xi}\boldsymbol{\xi} \rangle = \mathbf{s} \tag{1.1.23}$$

which is symmetric and non-negative definite. The surfaces of constant probability are elliptic hypersurfaces of second order. The variables $\boldsymbol{x}$ are called jointly normal.

All cumulants of higher than second order vanish. A principal-axes transformation diagonalizing s introduces "normal coordinates" which are not only uncorrelated but in this case statistically independent, as can be seen from the factorization of (1.1.21).

1.2. Stochastic processes

In the course of time, the state vector $\boldsymbol{x}$ of every member of the statistical ensemble will carry out a motion in state space Σ. The trajectory $\boldsymbol{x}(t)$ is called a *sample function* or *realization.* Any statistical ensemble of sample functions forms a *stochastic process.* For a fixed time t, the stochastic process is a random variable $\boldsymbol{x} \in \Sigma$ with probability distribution $p(\boldsymbol{x}t)$; for a pair of time instants $t^{(1)}$, $t^{(2)}$, one has two random variables $\boldsymbol{x}^{(1)}$, $\boldsymbol{x}^{(2)}$, with a *joint probability distribution* $p^{(2)}(\boldsymbol{x}^{(1)}t^{(1)}, \boldsymbol{x}^{(2)}t^{(2)})$, etc. The set of all possible sample functions $\boldsymbol{x}(t)$ forms a functional manifold Ω, and the stochastic process is a probability distribution in Ω. In order to avoid functional integration, we define the stochastic process by all its multiple-time joint probability distributions (multivariate distributions): For every $n = 1, 2, \ldots$ and every sequence of time instants $T = \{t^{(1)}, \ldots t^{(n)}\}$ there exists for the sequence of state vectors $\boldsymbol{X} = \{\boldsymbol{x}^{(1)}, \ldots \boldsymbol{x}^{(n)}\}$ a distribution $p^{(n)}(T) \in \Pi^*(\Sigma^n)$ with values

$$p^{(n)}(\boldsymbol{X}T) = p^{(n)}(\boldsymbol{x}^{(1)}t^{(1)}, \ldots \boldsymbol{x}^{(n)}t^{(n)}) \,. \tag{1.2.1}$$

The distribution $p^{(n)}(\boldsymbol{X}T)$ satisfies the symmetry relation

$$p^{(n)}(\boldsymbol{X}T) = p^{(n)}(\mathbb{P}(\boldsymbol{X}T)) \tag{1.2.2}$$

where $\mathbb{P}$ denotes a permutation of the n pairs $(\boldsymbol{x}^{(i)}t^{(i)})$.

The multivariate distributions $p^{(n)}$, $n = 1, 2, \ldots$ are not all independent of each other. In fact we have the compatibility relations

$$p^{(n)}(\boldsymbol{X}T) = \int p^{(n+k)}(\boldsymbol{X}T, \boldsymbol{Y}S)\, \mathrm{d}Y, \qquad n, k = 1, 2, \ldots \,. \tag{1.2.3}$$

We restrict the consideration to *stochastically continuous* processes with the property

$$p^{(n)}(\ldots x^{(i)}t^{(i)}, x^{(j)}t^{(j)}, \ldots) \to p^{(n-1)}(\ldots x^{(i)}t^{(i)}, \ldots)\, \delta(x^{(i)} - x^{(j)}) \qquad \text{for } t^{(i)} \to t^{(j)}. \tag{1.2.4}$$

A process is called *strictly stationary* if

$$p^{(n)}(X, T + \tau D) = p^{(n)}(XT) \qquad \forall \tau \tag{1.2.5}$$

where $D = (1, \ldots 1)$.

If one introduces a new state space $\Sigma^{(q)}$ according to (1.1.10), the stochastic process in $\Sigma^{(q)}$ is defined by the n-time multivariate distributions $p^{(n)}$ of the sequences $\boldsymbol{Q} = \{q^{(1)}, \ldots q^{(n)}\}$ of new state vectors, obtained from the original $p^{(n)}$ by

$$p^{(n)}(\boldsymbol{QT}) = \int \delta(Q(\boldsymbol{X}) - \boldsymbol{Q})\, p^{(n)}(\boldsymbol{XT})\, \mathrm{d}X. \tag{1.2.6}$$

Any random variable defined by a state function $f(\boldsymbol{xt})$ which may be explicitly time-dependent in general, represents a stochastic process consisting of sample functions $f(\boldsymbol{x}(t), t)$.* The mean value at time t is given by

$$\langle f(t) \rangle = \int f(\boldsymbol{xt})\, p(\boldsymbol{xt})\, \mathrm{d}x, \tag{1.2.7}$$

the *two-time correlation* between two processes $f(t)$ and $g(t)$ is obtained as

$$\langle f(s)\, g^*(t) \rangle = \int f(\boldsymbol{x}s)\, g^*(\boldsymbol{y}t)\, p^{(2)}(\boldsymbol{x}s, \boldsymbol{y}t)\, \mathrm{d}x\, \mathrm{d}y, \tag{1.2.8}$$

etc. The fluctuations

$$\varphi(t) = f(t) - \langle f(t) \rangle \tag{1.2.9}$$

of a set of random variables $f(t) = \{f_1(t), f_2(t), \ldots\}$ can be characterised by the two-time covariance matrix

$$\mathbf{S}(t_2, t_1) = \langle \varphi(t_2)\, \varphi^*(t_1) \rangle \equiv \langle f(t_2)\, f^*(t_1) \rangle - \langle f(t_2) \rangle \langle f^*(t_1) \rangle \tag{1.2.10}$$

with the autocorrelations $\langle \varphi_i(t_2)\, \varphi_i^*(t_1) \rangle$ as diagonal elements and the cross-correlations $\langle \varphi_i(t_2)\, \varphi_j^*(t_1) \rangle$ as nondiagonal elements. $\mathbf{S}(t_2, t_1)$ is a non-negative definite matrix kernel** [25] and satisfies

$$\mathbf{S}(t_2, t_1) = \mathbf{S}^\dagger(t_1, t_2). \tag{1.2.11}$$

* We denote both the sample functions and the random variables at a given time t by the same symbol $f(t)$. The specific meaning will be clear from the context.

** A matrix function $\mathbf{S}(t, t')$ is called a non-negative definite matrix kernel on $T \times T$, if for any n, any sequence of complex-valued vectors φ_i and any sequence of points $t_i (i = 1, \ldots n)$, one has $\Sigma_{i,j} \varphi_i^* \cdot \mathbf{S}(t_i, t_j) \cdot \varphi_j \geq 0$.

It is interesting to consider the Fourier transforms of the fluctuations $\varphi(t)$ with respect to time,

$$\varphi(\omega) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} \varphi(t) \exp(\mathrm{i}\omega t)\, \mathrm{d}t \tag{1.2.12}$$

$$\varphi(t) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} \varphi(\omega) \exp(-\mathrm{i}\omega t)\, \mathrm{d}\omega\,, \tag{1.2.13}$$

where the Fourier amplitude $\varphi(\omega)$ may contain δ-functions and their derivatives. The correlation matrix of the Fourier amplitudes

$$\mathbf{S}(\omega_2, \omega_1) = \langle \varphi(\omega_2)\, \varphi^*(\omega_1) \rangle \tag{1.2.14}$$

is the double Fourier transform of the two-time covariance matrix (generalized Wiener–Khintchin theorem)

$$\mathbf{S}(\omega_2, \omega_1) = (2\pi)^{-1} \int_{-\infty}^{+\infty} \int \mathbf{S}(t_2, t_1) \exp\{\mathrm{i}(\omega_2 t_2 - \omega_1 t_1)\}\, \mathrm{d}t_1\, \mathrm{d}t_2\,. \tag{1.2.15}$$

From (1.2.11) and (1.2.15), one concludes

$$\mathbf{S}(\omega_2, \omega_1) = \mathbf{S}^\dagger(\omega_1, \omega_2)\,. \tag{1.2.16}$$

Thus, the equal-frequency covariance matrix $\mathbf{S}(\omega, \omega)$ is Hermitian. Further, it can be shown that the double Fourier transforms of the autocorrelations $S_{ii}(t_2, t_1)$ satisfy [24]

$$\int_a^b \int_a^b S_{ii}(\omega_2, \omega_1)\, \mathrm{d}\omega_1\, \mathrm{d}\omega_2 \geq 0 \tag{1.2.17}$$

with arbitrary $a, b \in [-\infty, \infty]$. In particular, it follows that $S_{ii}(\omega, \omega) \geq 0$.

Of particular importance is the case that the covariance matrix $\mathbf{S}(t_2, t_1)$ becomes invariant against time translations,

$$\mathbf{S}(t_2, t_1) = \mathbf{S}(t_2 - t_1), \qquad \mathbf{S}(-\tau) = \mathbf{S}^\dagger(\tau)\,. \tag{1.2.18}$$

This is always the case for a strictly stationary process and random variables $\boldsymbol{f} = \{f_1, f_2, \ldots\}$ which are not explicitly time-dependent. As a consequence

$$\mathbf{S}(\omega_2, \omega_1) = \mathbf{S}(\omega_2)\, \delta(\omega_2 - \omega_1)\,, \tag{1.2.19}$$

where $\mathbf{S}(\omega)$ is the *spectral matrix* defined by

$$\mathbf{S}(\omega) = \int_{-\infty}^{+\infty} \mathbf{S}(\tau) \exp(\mathrm{i}\omega\tau)\, \mathrm{d}\tau = \mathbf{S}^{\dagger}(-\omega) \tag{1.2.20}$$

(Wiener–Khintchin theorem). From eqs. (1.2.18) and (1.2.20) it follows that $\mathbf{S}(\omega)$ is Hermitian and nonnegative definite. The diagonal elements $S_{ii}(\omega)$, which are called *spectral densities* or *power spectra* of the fluctuations φ_i, satisfy [24, 26]

$$S_{ii}(\omega) = S_{ii}(-\omega) = \int_{-\infty}^{+\infty} S_{ii}(\tau) \exp(\mathrm{i}\omega\tau)\, \mathrm{d}\tau \geq 0\,. \tag{1.2.21}$$

Moreover, $\mathbf{S}(\omega)$ can be diagonalized by a unitary transformation of the Fourier amplitudes $\varphi_i(\omega)$. The new variables are normal coordinates of the process in the sense that they are statistically decoupled up to second order in the fluctuations. The eigenvalues of $\mathbf{S}(\omega)$ are just the spectral densities of these normal coordinates.

The spectral matrix $\mathbf{S}(\omega)$ of the fluctuations is of great importance in linear transport theory and in scattering theory: It is connected with the dissipative part of the transport matrix by the famous fluctuation-dissipation theorem [7, 27, 28], and the spectral densities $S_{ii}(\omega)$ determine the cross-sections for scattering of light and neutrons by the fluctuations [29]. Further, as will be shown in section 5, the linear response of nonequilibrium systems is given by a generalized fluctuation theorem.

1.2.E1. Exponentially decaying correlations

As an example, we consider a process with an oscillating autocorrelation function with exponentially decaying amplitude,

$$S(\tau) = S_0 \cos\omega_0\tau \exp(-\gamma|\tau|), \qquad \gamma > 0\,. \tag{1.2.22}$$

The corresponding spectral density

$$S(\omega) = S_0\left[\frac{\gamma}{\gamma^2 + (\omega_0 - \omega)^2} + \frac{\gamma}{\gamma^2 + (\omega_0 + \omega)^2}\right] \tag{1.2.23}$$

is obviously positive (see fig. 1).

This example contains as limiting cases for $\gamma = 0$ the undamped oscillations with

$$S(\tau) = S_0 \cos\omega_0\tau \tag{1.2.24}$$

yielding

$$S(\omega) = S_0\,[\delta(\omega - \omega_0) + \delta(\omega + \omega_0)]\,, \tag{1.2.25}$$

and for $\gamma \to \infty$, $S_0 \to \infty$, $S_0/\gamma \to A/2$ the "white noise" with

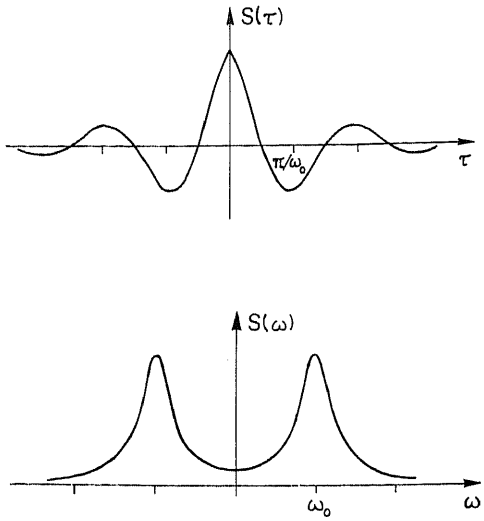

Fig. 1. Autocorrelation function $S(\tau)$ (1.2.22) and spectral density $S(\omega)$ (1.2.23).

$$S(\tau) = A\,\delta(\tau), \qquad A > 0\,, \tag{1.2.26}$$

and

$$S(\omega) = A\,. \tag{1.2.27}$$

1.3. Markov and non-Markov processes

In the theory of stochastic processes the concept of *conditional probability* plays an important role. Let $T = T_2 \cup T_1$ be a sequence of $m + n$ time instants with a corresponding sequence of state vectors $\boldsymbol{X} = \boldsymbol{X}_2 \cup \boldsymbol{X}_1$,

$$\begin{aligned} T_2 &= \{t_2^{(1)}, \ldots t_2^{(n)}\}, \qquad \boldsymbol{X}_2 = \{\boldsymbol{x}_2^{(1)}, \ldots \boldsymbol{x}_2^{(n)}\} \\ T_1 &= \{t_1^{(1)}, \ldots t_1^{(m)}\}, \qquad \boldsymbol{X}_1 = \{\boldsymbol{x}_1^{(1)}, \ldots \boldsymbol{x}_1^{(m)}\}\,, \end{aligned} \tag{1.3.1}$$

then the conditional probabilities $R^{(n|m)}$ are defined through

$$p^{(n+m)}(\boldsymbol{X}_2 T_2, \boldsymbol{X}_1 T_1) = R^{(n|m)}(\boldsymbol{X}_2 T_2 | \boldsymbol{X}_1 T_1)\, p^{(m)}(\boldsymbol{X}_1 T_1) \tag{1.3.2}$$

for state sequences $\boldsymbol{X}_1$ with $p^{(m)}(\boldsymbol{X}_1 T_1) \neq 0$. They have the properties

$$R^{(n+k|m)}(\boldsymbol{X}_2 T_2, \boldsymbol{Y}S | \boldsymbol{X}_1 T_1) = R^{(n|m+k)}(\boldsymbol{X}_2 T_2 | \boldsymbol{Y}S, \boldsymbol{X}_1 T_1)\, R^{(k|m)}(\boldsymbol{Y}S | \boldsymbol{X}_1 T_1)\,, \tag{1.3.3}$$

$$\int R^{(n+k|m)}(\boldsymbol{X}_2 T_2, \boldsymbol{Y}S | \boldsymbol{X}_1 T_1)\, \mathrm{d}Y = R^{(n|m)}(\boldsymbol{X}_2 T_2 | \boldsymbol{X}_1 T_1)\,, \tag{1.3.4}$$

and

$$\int R^{(n|m)}(\boldsymbol{X}_2 T_2|\boldsymbol{X}_1 T_1)\,\mathrm{d}X_2 = 1\,. \tag{1.3.5}$$

Further, for stochastically continuous processes

$$\lim_{T_2 \to T_1^{\uparrow}} R^{(n|n)}(\boldsymbol{X}_2 T_2|\boldsymbol{X}_1 T_1) = \delta(\boldsymbol{X}_2 - \boldsymbol{X}_1)\,. \tag{1.3.6}$$

We shall only use conditional probabilities with past conditions, where the largest $t_1 \in T_1$ is less than or equal to the smallest $t_2 \in T_2$.

Extending the notation introduced in (1.1.7,8), $p^{(n)}(T)$ denotes an element of function space $\Pi^{*}(\Sigma^n)$ with values $p^{(n)}(\boldsymbol{X}T)$. Elements like $R^{(n|m)}(T_2|T_1)$ are operators mapping $\Pi(\Sigma^m)$ on $\Pi(\Sigma^n)$ with kernels $R^{(n|m)}(\boldsymbol{X}_2 T_2|\boldsymbol{X}_1 T_1)$. Application of an operator to an element of $\Pi(\Sigma^k)$ and operator multiplication are written in the usual way as products $R^{(n|k)}(T|S)\,p^{(k)}(S)$ and $R^{(n|k)}(T_2|S)\,R^{(k|m)}(S|T_1)$, respectively,

$$[R^{(n|k)}(T|S)\,p^{(k)}(S)]_{\boldsymbol{X}} = \int R^{(n|k)}(\boldsymbol{X}T|\boldsymbol{Y}S)\,p^{(k)}(\boldsymbol{Y}S)\,\mathrm{d}Y \tag{1.3.7}$$

$$[R^{(n|k)}(T_2|S)R^{(k|m)}(S|T_1)]_{\boldsymbol{X}_2,\boldsymbol{X}_1} = \int R^{(n|k)}(\boldsymbol{X}_2 T_2|\boldsymbol{Y}S)\,R^{(k|m)}(\boldsymbol{Y}S|\boldsymbol{X}_1 T_1)\,\mathrm{d}Y\,. \tag{1.3.8}$$

With this notation, one obtains from (1.3.2) by integrating over $\boldsymbol{X}_1$ using (1.2.3)

$$p^{(n)}(T_2) = R^{(n|m)}(T_2|T_1)\,p^{(m)}(T_1)\,, \tag{1.3.9}$$

and eq. (1.3.6) for stochastically continuous processes takes the form

$$\lim_{T_2 \to T_1^{\uparrow}} R^{(n|n)}(T_2|T_1) = \mathbb{1}\,. \tag{1.3.10}$$

Eq. (1.3.3) yields after integration over $\boldsymbol{Y}$ and using (1.3.4) the balance equation for the conditional probabilities

$$R^{(n|m)}(T_2|T_1) = R^{(n|m+k)}(T_2|S, T_1)\,R^{(k|m)}(S|T_1) \tag{1.3.11}$$

valid for any stochastic process.

The most important class of stochastic processes are the *Markov processes* which satisfy

$$R^{(n|m)}(T_2|t_1^{(1)}, \ldots t_1^{(m)}) = R^{(n|1)}(T_2|t_1^{(1)}) \tag{1.3.12}$$

for any integers $n,m \geq 0$, where $t_1^{(1)}$ is the time instant of the latest condition, $t_1^{(1)} > t_1^{(i)}$, $i > 1$. Loosely speaking, the Markov principle states that the process has no memory of the past for a known present. As a consequence, all conditional probabilities $R^{(n|m)}$ can be expressed by repeated application of (1.3.3) with $k = 1$ in terms of the two-time conditional probability $R^{(1|1)}(t_2|t_1) = R(t_2|t_1)$

$$R^{(n|\ldots)}(x^{(1)}t^{(1)}, \ldots x^{(n)}t^{(n)}|x^{(n+1)}t^{(n+1)}, \ldots) = R(x^{(1)}t^{(1)}|x^{(2)}t^{(2)}) \cdots R(x^{(n)}t^{(n)}|x^{(n+1)}t^{(n+1)}) , \tag{1.3.13}$$

where $t^{(1)} > \cdots t^{(n)} > t^{(n+1)} > \cdots$. Thus, in the Markov case, the operator set $R(t|s)$ contains all the information necessary to calculate any multivariate distribution $p^{(n)}$ from the single-event distribution $p^{(1)} = p$ at a fixed time s: From (1.3.2) follows for $m = 1$ by using (1.3.13)

$$p^{(n)}(x^{(1)}t^{(1)}, \ldots x^{(n)}t^{(n)}) = R(x^{(1)}t^{(1)}|x^{(2)}t^{(2)}) \cdots R(x^{(n-1)}t^{(n-1)}|x^{(n)}t^{(n)})\, p(x^{(n)}t^{(n)}) . \tag{1.3.14}$$

It is important to note that a given operator set $R(t|s)$ generates a whole class C of stochastic processes from the set of different initial distributions $p(t_0)$. The term "Markov process" is often used to designate the whole class.

From the balance equation (1.3.11) we obtain with (1.3.12) for $n = k = 1$ the well-known *Chapman–Kolmogorov–Smoluchowski equation*

$$R(t_2|t_1) = R(t_2|s)\, R(s|t_1), \qquad t_2 \geq s \geq t_1 . \tag{1.3.15}$$

The $R(t_2|t_1)$ act as propagators for the time evolution of the single-event probability p: From (1.3.14) follows for $n = 1$ by integration over y

$$p(t_2) = R(t_2|t_1)\, p(t_1) . \tag{1.3.16}$$

If the conditional probabilities $R(t_2|t_1)$ are invariant against arbitrary time translations τ,

$$R(t_2 + \tau|t_1 + \tau) = R(t_2|t_1) = R(t_2 - t_1) , \tag{1.3.17}$$

the Markov process is called *time-homogeneous*, and the propagators set $\{R(\tau)\}$ forms a semigroup. For such a process, the probability distributions $p(t)$, $p^{(2)}(t + \tau, t)$ etc. may still depend on time t.

For *a non-Markov process*, the conditional probabilities $R(t_2|t_1)$ in general do not satisfy the Chapman–Kolmogorov–Smoluchowski equation (1.3.15), and the conditional probabilities depend on previous history. We have shown [30] that even in this case the time evolution of all multivariate distributions can be described in terms of n-parameter propagator sets $G^{(n)}(T_2|T_1)$ such that

$$p^{(n)}(T_2) = G^{(n|n)}(T_2|T_1)\, p^{(n)}(T_1) . \tag{1.3.18}$$

But these propagators are different from the conditional probabilities, and can therefore not be used to calculate $p^{(2n)}(T_2 \cup T_1)$.

We illustrate these concepts by three examples, the two-state process, the Gauss process, and the process with independent increments.

1.3.E1. The two-state process

The joint probability $p^{(2)}$ of a two-state process of the Ising variable $x(t) = \pm 1$ can be written

$$p^{(2)}(x_2t_2, x_1t_1) = \tfrac{1}{4}[1 + a(t_2)\, x_2 + a(t_1)\, x_1 + r(t_2, t_1)\, x_2x_1] . \tag{1.3.19}$$

It is completely determined by the mean values

$$\langle x(t_{2,1})\rangle = a(t_{2,1}) \tag{1.3.20}$$

and the autocorrelation function

$$\langle x(t_2)\, x(t_1)\rangle = r(t_2, t_1)\,. \tag{1.3.21}$$

The variance and the two-time auto-covariance of the fluctuations $\xi(t) = x(t) - a(t)$ are given by

$$\langle \xi^2(t)\rangle \equiv s(t) = 1 - a^2(t) \tag{1.3.22}$$

and

$$\langle \xi(t_2)\, \xi(t_1)\rangle \equiv s(t_2, t_1) = r(t_2, t_1) - a(t_2)\, a(t_1)\,, \tag{1.3.23}$$

respectively. The conditional probability $R(t_2|t_1)$ has the form*

$$R(x_2 t_2|x_1 t_1) = \tfrac{1}{2}\{1 + x_2[\alpha(t_2, t_1) + \rho(t_2, t_1)\, x_1]\}\,, \tag{1.3.24}$$

where $\alpha(t_2, t_1)$ and $\rho(t_2, t_1)$ obey

$$|\alpha(t_2, t_1) \pm \rho(t_2, t_1)| \leq 1\,. \tag{1.3.25}$$

These quantities determine the propagation of $a(t)$ and $r(t_2, t_1)$: From (1.3.2) for $m = n = 1$ one obtains

$$a(t_2) = \alpha(t_2, t_1) + \rho(t_2, t_1)\, a(t_1) \tag{1.3.26}$$

$$r(t_2, t_1) = \rho(t_2, t_1) + \alpha(t_2, t_1)\, a(t_1), \tag{1.3.27}$$

from which it follows that

$$s(t_2, t_1) = \rho(t_2, t_1)\, s(t_1), \qquad t_2 \geq t_1\,. \tag{1.3.28}$$

For a stochastically continuous process one has

$$\rho(t^+, t) = 1\,, \qquad \alpha(t^+, t) = 0\,, \tag{1.3.29}$$

yielding

$$R(x_2 t|x_1 t) = \tfrac{1}{2}(1 + x_1 x_2) \equiv \delta_{x_1, x_2}\,. \tag{1.3.30}$$

* $R(xt|ys)$ is the kernel of an operator $R(t|s)$ which may be expressed in terms of the unit matrix $\mathbb{1}$ and the Pauli matrices $\sigma_{1,2,3}$ as

$$R(t|s) = \tfrac{1}{2}\{[1 + \rho(t, s)]\, \mathbb{1} + [1 - \rho(t, s)]\, \sigma_1 + \alpha(t, s)\, (\sigma_3 - i\sigma_2)\}\,.$$

When the process is Markovian, the Chapman–Kolmogorov–Smoluchowski equation (1.3.15) implies that $\rho(t_2, t_1)$ and $\alpha(t_2, t_1)$ satisfy

$$\rho(t_2, t_1) = \rho(t_2, s)\,\rho(s, t_1) \tag{1.3.31}$$

$$\alpha(t_2, t_1) = \alpha(t_2, s) + \rho(t_2, s)\,\alpha(s, t_1) \tag{1.3.32}$$

for all $t_1 \leq s \leq t_2$. For a stochastically continuous two-state Markov process, $\rho(t_2, t_1)$ is strictly positive,

$$\rho(t_2, t_1) > 0 \qquad \forall t_1 \leq t_2 < \infty\,. \tag{1.3.33}$$

This can be seen by the following argument: Since $\rho(t^+, t) = 1$, $\rho(t, t_1)$ must be positive at least in a certain interval. Assume that $\rho(t, t_1) > 0$ for $t_1 \leq t < t_2$ and $\rho(t_2, t_1) = 0$. Then it follows from (1.3.31) that $\rho(t_2, s) = 0$ for all s satisfying $t_1 \leq s \leq t_2$, which is in contradiction with the requirement $\rho(t_2, t_2^-) = 1$.

The process is time-homogeneous if

$$\rho(t_2, t_1) = \rho(t_2 - t_1), \qquad \alpha(t_2, t_1) = \alpha(t_2 - t_1), \qquad t_2 \geq t_1\,. \tag{1.3.34}$$

For a time-homogeneous process, the Markov conditions (1.3.31, 32) take the form

$$\rho(\tau_1 + \tau_2) = \rho(\tau_1)\,\rho(\tau_2) \tag{1.3.35}$$

$$\alpha(\tau_1 + \tau_2) = \alpha(\tau_1) + \rho(\tau_1)\,\alpha(\tau_2)\,. \tag{1.3.36}$$

If the process is stationary in the strict sense, it has to satisfy in addition

$$\alpha(\tau) = (1 - \rho(\tau))\,a\,, \qquad \tau \geq 0 \tag{1.3.37}$$

with $a = \text{const.}$, whence

$$\dot{\alpha}(\tau) = -\dot{\rho}(\tau)\,a\,, \tag{1.3.38}$$

if the process is stochastically differentiable (see section 2.2).

1.3.E2. The n-component Gauss process

A real n-component Gauss process $\boldsymbol{x}(t)$ has the k-time joint probability distributions ($k = 1, 2, \ldots$)

$$p^{(k)}(\boldsymbol{x}_1 t_1, \ldots \boldsymbol{x}_k t_k) = \det(2\pi \mathbf{S}^{(k)})]^{-1/2} \exp\left\{-\tfrac{1}{2} \sum_{i,j=1}^{k} (\boldsymbol{x}_i - \boldsymbol{a}(t_i)) \cdot (\mathbf{S}^{(k)-1})_{ij} \cdot (\boldsymbol{x}_j - \boldsymbol{a}(t_j))\right\} \tag{1.3.39}$$

which are completely determined by the vector of mean values

$$\langle \boldsymbol{x}(t_i) \rangle = \boldsymbol{a}(t_i) \tag{1.3.40}$$

and the $(n \times n)$ two-time covariance matrices of the fluctuations $\boldsymbol{\xi}(t) = \boldsymbol{x}(t) - \boldsymbol{a}(t)$,

$$\langle \xi(t_i)\, \xi(t_j)\rangle = \mathbf{s}(t_i, t_j), \qquad \mathbf{s}(t_i, t_i) \equiv \mathbf{s}(t_i) \tag{1.3.41}$$

forming the blocks of the symmetric non-negative definite $(kn)\times(kn)$ matrix $\mathbf{S}^{(k)}$.*

The conditional probability $R(t_2|t_1)$

$$R(x_2t_2|x_1t_1) = [\det(2\pi\boldsymbol{\sigma}(t_2, t_1))]^{-1/2} \exp\{-\tfrac{1}{2}[x_2 - (\boldsymbol{\rho}(t_2, t_1)\cdot x_1 + \boldsymbol{\alpha}(t_2, t_1))]\cdot\boldsymbol{\sigma}^{-1}(t_2, t_1)\cdot[x_2 - (\boldsymbol{\rho}(t_2, t_1)\cdot x_1 + \boldsymbol{\alpha}(t_2, t_1))]\} \tag{1.3.42}$$

is determined by the matrix $\boldsymbol{\sigma}(t_2, t_1)$,

$$\boldsymbol{\sigma}(t_2, t_1) = \boldsymbol{\sigma}^{\dagger}(t_2, t_1) \text{ non-negative definite,} \tag{1.3.43}$$

the matrix $\boldsymbol{\rho}(t_2, t_1)$, and the vector $\boldsymbol{\alpha}(t_2, t_1)$. These quantities determine the propagation of the covariance matrix $\mathbf{S}^{(2)} \equiv \mathbf{S}(t_2, t_1)$ and the vector of mean values $a(t)$. From (1.3.2) for $m = n = 1$ one finds

$$a(t_2) = \boldsymbol{\alpha}(t_2, t_1) + \boldsymbol{\rho}(t_2, t_1)\cdot a(t_1) \tag{1.3.44}$$

and an expression for $\mathbf{S}^{-1}(t_2, t_1)$ which can be factorized,

$$\mathbf{S}^{-1}(t_2, t_1) = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ -\boldsymbol{\rho}^{\dagger}(t_2, t_1) & \mathbf{s}^{-1}(t_1) \end{pmatrix}\cdot\begin{pmatrix} \boldsymbol{\sigma}^{-1}(t_2, t_1) & -\boldsymbol{\sigma}^{-1}(t_2, t_1)\cdot\boldsymbol{\rho}(t_2, t_1) \\ \mathbf{0} & \mathbf{1} \end{pmatrix}, \tag{1.3.45}$$

and is easily inverted to give

$$\mathbf{s}(t_2) = \boldsymbol{\sigma}(t_2, t_1) + \boldsymbol{\rho}(t_2, t_1)\cdot\mathbf{s}(t_1)\cdot\boldsymbol{\rho}^{\dagger}(t_2, t_1), \tag{1.3.46}$$

$$\mathbf{s}(t_2, t_1) = \boldsymbol{\rho}(t_2, t_1)\cdot\mathbf{s}(t_1) \tag{1.3.47}$$

and

$$\det \mathbf{S} = \det \boldsymbol{\sigma}(t_2, t_1)\det \mathbf{s}(t_1). \tag{1.3.48}$$

For a stochastically continuous process one has

$$\boldsymbol{\rho}(t^+, t) = \mathbf{1}, \qquad \boldsymbol{\sigma}(t^+, t) = 0, \qquad \boldsymbol{\alpha}(t^+, t) = 0. \tag{1.3.49}$$

For a Markov process, the relations

$$\boldsymbol{\rho}(t_2, t_1) = \boldsymbol{\rho}(t_2, s)\cdot\boldsymbol{\rho}(s, t_1) \tag{1.3.50}$$

$$\boldsymbol{\alpha}(t_2, t_1) = \boldsymbol{\alpha}(t_2, s) + \boldsymbol{\rho}(t_2, s)\cdot\boldsymbol{\alpha}(s, t_1) \tag{1.3.51}$$

$$\boldsymbol{\sigma}(t_2, t_1) = \boldsymbol{\sigma}(t_2, s) + \boldsymbol{\rho}(t_2, s)\cdot\boldsymbol{\sigma}(s, t_1)\cdot\boldsymbol{\rho}^{\dagger}(t_2, s) \tag{1.3.52}$$

* Note that for fixed times $\{t_1, \ldots t_k\}$, (1.3.39) is a (kn)-component Gaussian distribution (1.1.21) with $\mathbf{S}^{(k)}$ as covariance matrix (see (1.1.23)).

have to be satisfied for all $t_1 \leq s \leq t_2$. These conditions are also sufficient to guarantee that the Gauss process (1.3.39) is Markovian (Doob's theorem [2, 40]).

For a stochastically continuous Gauss–Markov process,

$$\boldsymbol{\rho}(t_2, t_1) \text{ non-singular } \forall t_1 \leq t_2 < \infty, \tag{1.3.53}$$

which can be seen by the same argument as given for (1.3.33), applied to det $\boldsymbol{\rho}(t_2, t_1)$.

The process is time-homogeneous if

$$\boldsymbol{\rho}(t_2, t_1) = \boldsymbol{\rho}(t_2 - t_1) \tag{1.3.54}$$

$$\boldsymbol{\alpha}(t_2, t_1) = \boldsymbol{\alpha}(t_2 - t_1) \tag{1.3.55}$$

$$\boldsymbol{\sigma}(t_2, t_1) = \boldsymbol{\sigma}(t_2 - t_1). \tag{1.3.56}$$

For a time-homogeneous process, the Markov conditions (1.3.50–52) take the form

$$\boldsymbol{\rho}(\tau_1 + \tau_2) = \boldsymbol{\rho}(\tau_1) \cdot \boldsymbol{\rho}(\tau_2) \tag{1.3.57}$$

$$\boldsymbol{\alpha}(\tau_1 + \tau_2) = \boldsymbol{\alpha}(\tau_1) + \boldsymbol{\rho}(\tau_1) \cdot \boldsymbol{\alpha}(\tau_2) \tag{1.3.58}$$

$$\boldsymbol{\sigma}(\tau_1 + \tau_2) = \boldsymbol{\sigma}(\tau_1) + \boldsymbol{\rho}(\tau_1) \cdot \boldsymbol{\sigma}(\tau_2) \cdot \boldsymbol{\rho}^{\dagger}(\tau_1). \tag{1.3.59}$$

If the process is stationary in the strict sense, it has to satisfy in addition

$$\boldsymbol{\alpha}(\tau) = (\mathbf{1} - \boldsymbol{\rho}(\tau)) \cdot \boldsymbol{a} \tag{1.3.60}$$

and (see (1.3.46))

$$\boldsymbol{\sigma}(\tau) = \mathbf{s} - \boldsymbol{\rho}(\tau) \cdot \mathbf{s} \cdot \boldsymbol{\rho}^{\dagger}(\tau) \tag{1.3.61}$$

with $\boldsymbol{a}$ = const., $\mathbf{s}$ = const., whence

$$\dot{\boldsymbol{\alpha}}(\tau) = -\dot{\boldsymbol{\rho}}(\tau) \cdot \boldsymbol{a} \tag{1.3.62}$$

$$\dot{\boldsymbol{\sigma}}(\tau) = -\dot{\boldsymbol{\rho}}(\tau) \cdot \mathbf{s} \cdot \boldsymbol{\rho}^{\dagger}(\tau) - \boldsymbol{\rho}(\tau) \cdot \mathbf{s} \cdot \dot{\boldsymbol{\rho}}^{\dagger}(\tau) \tag{1.3.63}$$

if the process is stochastically differentiable (see section 2.2).

An important and simple case of a time-homogeneous but nonstationary Gauss–Markov process is the one-component *Wiener process* with

$$\rho(\tau) = 1, \qquad \alpha(\tau) = 0, \qquad \sigma(\tau) = \tau, \tag{1.3.64}$$

i.e.

$$R(x\tau|y0) = \frac{1}{\sqrt{2\pi\tau}} \exp\left[-\frac{(x-y)^2}{2\tau}\right]. \tag{1.3.65}$$

The time evolution of the mean value $a(t)$ and the variance $s(t)$ are found from (1.3.44, 46),

$$a(t) = a(0), \qquad s(t) = t + s(0). \tag{1.3.66}$$

1.3.E3. Process with independent increments

We consider a process defined by a conditional probability

$$R(\boldsymbol{x}_2 t_2 | \boldsymbol{x}_1 t_1) = R(\boldsymbol{x}_2 - \boldsymbol{x}_1; t_2, t_1) \tag{1.3.67}$$

depending only on the increment $\boldsymbol{r} = \boldsymbol{x}_2 - \boldsymbol{x}_1$, i.e. the probability for an increment $\boldsymbol{r}$ to occur during $t_2 - t_1$ is independent of the starting point $\boldsymbol{x}_1$. Thus, the two-time joint probability $p^{(2)}$ has the structure

$$p^{(2)}(\boldsymbol{x}_2 t_2, \boldsymbol{x}_1 t_1) = R(\boldsymbol{x}_2 - \boldsymbol{x}_1; t_2, t_1)\, p^{(1)}(\boldsymbol{x}_1 t_1). \tag{1.3.68}$$

The object is to derive propagation equations for the mean value $\boldsymbol{a}(t) = \langle \boldsymbol{x}(t) \rangle$ and the equal-time covariance matrix $\mathbf{s}(t) = \langle \boldsymbol{\xi}(t)\, \boldsymbol{\xi}(t) \rangle$ of the fluctuations $\boldsymbol{\xi}(t) = \boldsymbol{x}(t) - \boldsymbol{a}(t)$. One obtains from (1.3.68)

$$\boldsymbol{a}(t_2) = \boldsymbol{\alpha}(t_2, t_1) + \boldsymbol{a}(t_1) \tag{1.3.69}$$

$$\mathbf{s}(t_2) = \boldsymbol{\sigma}(t_2, t_1) + \mathbf{s}(t_1) \tag{1.3.70}$$

where

$$\boldsymbol{\alpha}(t_2, t_1) = \int \boldsymbol{r}\, R(\boldsymbol{r}; t_2, t_1)\, \mathrm{d}\boldsymbol{r} \equiv \langle \boldsymbol{x}(t_2) | 0 t_1 \rangle \tag{1.3.71}$$

and

$$\boldsymbol{\sigma}(t_2, t_1) = \int \boldsymbol{r}\boldsymbol{r}\, R(\boldsymbol{r}; t_2, t_1)\, \mathrm{d}\boldsymbol{r} - \boldsymbol{\alpha}(t_2, t_1)\, \boldsymbol{\alpha}(t_2, t_1) \equiv \langle \boldsymbol{\xi}(t_2)\, \boldsymbol{\xi}(t_2) | 0 t_1 \rangle \tag{1.3.72}$$

are the conditional mean increment and the conditional covariance matrix, respectively. The two-time autocovariance matrix satisfies

$$\mathbf{s}(t_2, t_1) \equiv \langle \boldsymbol{\xi}(t_2)\, \boldsymbol{\xi}(t_1) \rangle = \mathbf{s}(t_1), \tag{1.3.73}$$

which is an immediate consequence of the independence of the increment $\boldsymbol{\xi}_2 - \boldsymbol{\xi}_1$ of the starting point $\boldsymbol{\xi}_1$.

In general, the probability (1.3.67) for an increment $\boldsymbol{r}$ to occur during $t_2 - t_1$, although independent of the starting point at t_1, may still depend on the previous history. If it is independent of previous history, i.e. if the process is Markovian, $\boldsymbol{\alpha}(t_2, t_1)$ and $\boldsymbol{\sigma}(t_2, t_1)$ satisfy

$$\boldsymbol{\alpha}(t_2, t_1) = \boldsymbol{\alpha}(t_2, s) + \boldsymbol{\alpha}(s, t_1) \tag{1.3.74}$$

and

$$\boldsymbol{\sigma}(t_2, t_1) = \boldsymbol{\sigma}(t_2, s) + \boldsymbol{\sigma}(s, t_1) \tag{1.3.75}$$

for all $t_1 \leq s \leq t_2$.

The process is time-homogeneous if $\boldsymbol{\alpha}$ and $\boldsymbol{\sigma}$ depend only on $t_2 - t_1 = \tau$. For a time-homogeneous process, the Markov conditions (1.3.76, 77) take the form

$$\boldsymbol{\alpha}(\tau_1 + \tau_2) = \boldsymbol{\alpha}(\tau_1) + \boldsymbol{\alpha}(\tau_2) \tag{1.3.76}$$

$$\boldsymbol{\sigma}(\tau_1 + \tau_2) = \boldsymbol{\sigma}(\tau_1) + \boldsymbol{\sigma}(\tau_2)\,, \tag{1.3.77}$$

whence

$$\boldsymbol{\alpha}(\tau) = \dot{\boldsymbol{\alpha}} \cdot \tau, \qquad \boldsymbol{\sigma}(\tau) = \dot{\boldsymbol{\sigma}} \cdot \tau \tag{1.3.78}$$

with $\dot{\boldsymbol{\alpha}} = \text{const.}$, $\dot{\boldsymbol{\sigma}} = \text{const.}$, if the process is stochastically differentiable (see section 2.2).

A Gauss process with $\boldsymbol{\rho}(t_2, t_1) = \mathbf{1}$ is a process with independent increments, and can be checked easily to satisfy the above relations.

2. Time evolution of stochastic processes

2.1. Microscopic origin of stochastic time evolution

The microscopic dynamics of the system is governed by the classical or quantum-mechanical Liouville–von Neumann equation of motion for the microscopic phase-space distribution or the microscopic statistical operator, respectively, for the total system (reservoirs included). Time-evolution equations for the statistical multivariate distributions $p^{(n)}$ in the space Σ of coarse-grained macrovariables $\boldsymbol{x}$ of the system can be constructed by eliminating the microscopic degrees of freedom of the system and the reservoirs with the help of projection-operator methods. This has been carried out for the single-event distribution $p^{(1)}$ [13, 18, 31, 32] resulting in the Nakajima–Zwanzig master equation

$$\dot{p}(t) = \int_{t_0}^{t} \Lambda(t|s)\, p(s)\, \mathrm{d}s + I(t)\,. \tag{2.1.1}$$

Here, the "retarded kernel" $\Lambda(t|s)$ is an operator acting on space $\Pi^*(\Sigma)$, which describes the memory effect of the distribution at time s on the rate of change at the later time t, caused by the elimination of the microscopic degrees of freedom. In general, $\Lambda(t|s)$ may contain an instantaneous contribution $\Gamma(t)\,\delta(t - s - 0^+)$. The inhomogeneous term $I(t)$ contains the effects of the preparation procedure and depends explicitly on the initial microdistribution at time t_0 of preparation. If the physical preparation procedure π, i.e. the initial distribution over the microstates belonging to a given macrostate, is explicitly taken into account in the definition of the projection operator, one can construct an exact master equation without the inhomogeneous term $I(t)$, with a uniquely defined preparation-dependent kernel $\Lambda_\pi(t|s)$ [33, 34].

Similar memory effects are present in the time-evolution equations for higher multivariate dis-

tributions $p^{(n)}(t^{(1)}, \ldots t^{(n)})$. Moreover, it is found that the memory kernels for $n > 1$ depend in general on the whole process σ under consideration, i.e. not only on the initial distribution over the microstates belonging to a given macrostate but also on the initial macrodistribution $p(t_0)$ [33, 34]. It is this fact (and *not* the retardation in the master equation (2.1.1) for the single-event distribution*) which clearly demonstrates the non-Markovian character of the macroprocess.

Evolution equations for conditional and joint probabilities are important not only for the calculation of time-correlation functions, but also as a starting point for a rigorous discussion of the Markovian limit. In order to obtain a Markov process, the operator determining the time evolution must become independent of the initial macrodistribution. This is expected to occur on a macroscopic time scale if the actual "non-Markovian" memory decays on a microscopic time scale τ^{micro} much shorter than the times characteristic for the macroscopic motion in state space Σ, i.e. if the variables of the system separate into two classes: One class consisting of all the approximately conserved quantities of the system, which change on a time scale much longer than the relaxation times of the remaining variables forming the second class. For the validity of the Markov approximation it is essential that all the variables of the first class are contained in the set $\boldsymbol{x}$ of macrovariables.

Such a "coarse-graining in time" over τ^{micro} leading to a Markov description simplifies the stochastic calculus enormously, because the Greens function $G(t|s)$, $t \geq s$ of a Markovian single-event master equation coincides with the conditional probability $R(t|s)$ of the process, and thus according to (1.3.14) all multivariate distributions $p^{(n)}(t^{(1)}, \ldots t^{(n)})$ are completely determined by the single-event master equation and the initial macrodistribution $p(t_0)$ alone. In the general non-Markov case, on the other hand, a separate evolution equation is required for each of the multivariate distributions [34].

In this review, we restrict the general presentation to the Markov case. A brief outlook on the non-Markov case is given in section 2.6.

2.2. Time evolution of Markov processes

In this subsection we study the differential equations governing the time evolution of a Markov process. According to the Chapman–Kolmogorov–Smoluchowski equation (1.3.15) the $R(t|s)$ form a propagator set. This set can be generated from the infinitesimal propagator

$$R(t + \mathrm{d}t|t) = \mathbb{1} + \Gamma(t)\,\mathrm{d}t, \qquad \mathrm{d}t > 0 \tag{2.2.1}$$

where the generator $\Gamma(s)$ of the set is defined by

$$\Gamma(s) = \frac{\mathrm{d}}{\mathrm{d}t} R(t|s)|_{t=s^+} = -\frac{\mathrm{d}}{\mathrm{d}s} R(t|s)|_{t=s^+} . \tag{2.2.2}$$

A process for which the derivatives of $R(t|s)$ exist will be called *stochastically differentiable.*

From the propagator property

$$R(t + \mathrm{d}t|s) = R(t + \mathrm{d}t|t)\, R(t|s), \qquad \mathrm{d}t > 0, \tag{2.2.3}$$

we find the *forward equation* [38–41]

* The retarded single-event master equation (2.1.1) may under fairly general conditions (nonsingularity of the Greens function) be formally recast into a time-convolutionless (but not memoryless!) form [33–37].

$$\frac{\mathrm{d}}{\mathrm{d}t} R(t|s) = \Gamma(t)\, R(t|s), \qquad t > s, \tag{2.2.4}$$

which involves differentiation with respect to the later time t. In a similar way we get from

$$R(t|s) = R(t|s + \mathrm{d}s)\, R(s + \mathrm{d}s|s), \qquad \mathrm{d}s > 0, \tag{2.2.5}$$

the equation

$$\frac{\mathrm{d}}{\mathrm{d}s} R(t|s) = -R(t|s)\, \Gamma(s), \qquad t > s, \tag{2.2.6}$$

involving differentiation with respect to the former time s. In terms of the transposed* operator $R^{\dagger}$, this becomes the *backward equation* [38–41]

$$\frac{\mathrm{d}}{\mathrm{d}s} R^{\dagger}(t|s) = -\Gamma^{\dagger}(s)\, R^{\dagger}(t|s), \qquad t > s. \tag{2.2.7}$$

Eqs. (2.2.4) and (2.2.6) show that the generator $\Gamma(t)$ determines the time evolution of a Markov process in the same sense as the Hamiltonian determines the time evolution of a Hamiltonian system. It will be called the *master operator*** of the process.

The formal solution of the forward equation can be written

$$R(t|t_1) = \mathcal{T} \exp \int_{t_1}^{t} \Gamma(s)\, \mathrm{d}s, \tag{2.2.8}$$

where $\mathcal{T}$ is the usual time-ordering operator. From this form, the propagator property (1.3.15) can immediately be read off.

For a time-homogeneous process, the master operator

$$\Gamma = \frac{\mathrm{d}}{\mathrm{d}\tau} R(\tau)\big|_{\tau = 0^+} \tag{2.2.9}$$

is independent of time, and the forward equation takes the form

$$\frac{\mathrm{d}}{\mathrm{d}\tau} R(\tau) = \Gamma R(\tau), \tag{2.2.10}$$

which has the solution

$$R(\tau) = \exp(\Gamma\tau). \tag{2.2.11}$$

* The kernels of R and $R^{\dagger}$ are related by $R^{\dagger}(x t|y s) = R(y t|x s)$.

** In this review, we use the term "master operator" to denote the generator of time evolution of any Markov process. Thus, the Fokker–Planck operator is a special case of a master operator and the Fokker–Planck equation a special case of a master equation.

The forward and backward equations have also the significance of equations of motion of the single-event probability $p(t)$ and of conditional expectations, respectively. By applying both sides of eq. (2.2.4) to $p(s)$ one obtains

$$\mathrm{d}p(t)/\mathrm{d}t = \Gamma(t)\, p(t)\,, \tag{2.2.12}$$

showing that $p(t)$ is a solution of the forward equation. This equation for $p(t)$ will be referred to as *master equation.* The conditional expectation $\langle f(t)|ys\rangle$ of a bounded state function $f(xt)$ is defined as the mean taken over the subset of sample functions passing through state y at the former time s,

$$\langle f(t)|ys\rangle = \int f(xt)\, R(xt|ys)\, \mathrm{d}x, \qquad t > s\,. \tag{2.2.13}$$

It can be considered as a state function of the condition y, and therefore as an element $\langle f(t)|s\rangle$ of function space $II(\Sigma)$. Therefore, using the convention introduced in (1.1.7), eq. (2.2.13) can be written

$$\langle f(t)|s\rangle = f(t)\, R(t|s) = R^{\dagger}(t|s)\, f(t) \tag{2.2.14}$$

whence

$$\frac{\mathrm{d}}{\mathrm{d}s}\langle f(t)|s\rangle = -\Gamma^{\dagger}(s)\,\langle f(t)|s\rangle\,. \tag{2.2.15a}$$

For a time-homogeneous process and f not explicitly time-dependent, this takes the form

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\langle f(\tau)|0\rangle = \Gamma^{\dagger}\langle f(\tau)|0\rangle\,. \tag{2.2.15b}$$

Thus, conditional averages are solutions of the backward equation with respect to their dependence on the time s of the condition. With respect to the time t of observation, on the other hand, they satisfy the same equation as any average $\langle f(t)\rangle$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle f(t)\rangle = \left\langle \Gamma^{\dagger}(t)\, f(t) + \frac{\partial}{\partial t} f(t)\right\rangle, \tag{2.2.16}$$

which will be of importance in the theory of stochastic differential equations (section 2.4).

2.2.E1. Time evolution of the two-state Markov process

For a stochastically differentiable two-state process, one obtains from (1.3.24) and (2.2.2) the master-operator kernel

$$\Gamma(x, y; t) = \tfrac{1}{2}x[\dot{\alpha}_0(t) + \dot{\rho}_0(t)\, y]\,, \tag{2.2.17}$$

where

$$\dot{\rho}_0(t) = \frac{\mathrm{d}}{\mathrm{d}s}\rho(s,t)|_{s=t^+}, \qquad \dot{\alpha}_0(t) = \frac{\mathrm{d}}{\mathrm{d}s}\alpha(s,t)|_{s=t^+}. \tag{2.2.18}$$

$\Gamma(x, y; t)$ is the kernel of an operator which may be expressed in terms of the unit matrix $\mathbb{1}$ and the Pauli matrices $\sigma_{1,2,3}$ as (compare footnote on p. 221)

$$\Gamma(t) = \tfrac{1}{2}[\dot{\rho}_0(t)(\mathbb{1} - \sigma_1) + \dot{\alpha}_0(t)(\sigma_3 - \mathrm{i}\sigma_2)]. \tag{2.2.19}$$

From (1.3.25) it follows that

$$\dot{\rho}_0(t) \leq 0, \qquad |\dot{\alpha}_0(t)| \leq |\dot{\rho}_0(t)|. \tag{2.2.20}$$

The quantities $\dot{\rho}_0$ and $\dot{\alpha}_0$ are related to the transition rates $w(1\to 2) = w_{21}$ and $w(2\to 1) = w_{12}$ (see section 2.3) by

$$\dot{\rho}_0 = -w_{21} - w_{12}, \qquad \dot{\alpha}_0 = -w_{21} + w_{12}. \tag{2.2.21}$$

For the time evolution of the mean value $a(t)$, one obtains from (1.3.26) the differential equation

$$\mathrm{d}a(t)/\mathrm{d}t = \dot{\alpha}_0(t) + \dot{\rho}_0(t)\, a(t). \tag{2.2.22}$$

For a Markov process, $\dot{\rho}_0(t)$ and $\dot{\alpha}_0(t)$ determine the time evolution of the quantities $\rho(t, t_1)$ and $\alpha(t, t_1)$. From the Markov conditions (1.3.31, 32) one obtains the differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t, t_1) = \dot{\rho}_0(t)\,\rho(t, t_1) \tag{2.2.23}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\alpha(t, t_1) = \dot{\alpha}_0(t) + \dot{\rho}_0(t)\,\alpha(t, t_1) \tag{2.2.24}$$

which have the solutions

$$\rho(t, t_1) = \exp\Big[\int_{t_1}^{t} \dot{\rho}_0(s)\,\mathrm{d}s\Big] \tag{2.2.25}$$

$$\alpha(t, t_1) = \int_{t_1}^{t} \rho(t, s)\,\dot{\alpha}_0(s)\,\mathrm{d}s. \tag{2.2.26}$$

For a stationary process, it follows from (2.2.22) that $\dot{\rho}_0 = \text{const.}$ and $\dot{\alpha}_0 = \text{const.}$ are related by

$$\dot{\alpha}_0 + \dot{\rho}_0 a = 0. \tag{2.2.27}$$

The solutions of the differential Markov conditions (2.2.23, 24) take the form

$$\rho(\tau) = \exp(\dot{\rho}_0 \tau) \tag{2.2.28}$$

and, using (2.2.27),

$$\alpha(\tau) = [1 - \exp(\dot{\rho}_0 \tau)]a \tag{2.2.29}$$

in agreement with (1.3.37).

2.2.E2. Time evolution of the Gauss–Markov process

The conditional probability $R(\boldsymbol{x}t|\boldsymbol{y}t_1)$ in (1.3.42) depends on t only via the quantities $\boldsymbol{\rho}(t, t_1)$, $\boldsymbol{\alpha}(t, t_1)$ and $\boldsymbol{\sigma}(t, t_1)$. Since

$$\frac{\partial R}{\partial \boldsymbol{\rho}} = -\frac{\partial R}{\partial \boldsymbol{x}}\boldsymbol{y}; \qquad \frac{\partial R}{\partial \boldsymbol{\alpha}} = -\frac{\partial R}{\partial \boldsymbol{x}}; \qquad \frac{\partial R}{\partial \boldsymbol{\sigma}} = \frac{1}{2}\frac{\partial^2 R}{\partial \boldsymbol{x}\,\partial \boldsymbol{x}}, \tag{2.2.30}$$

one obtains from (2.2.2) by observing (1.3.6) the master-operator kernel

$$\Gamma(\boldsymbol{x}, \boldsymbol{y}; t) = -[\dot{\boldsymbol{\rho}}_0(t) \cdot \boldsymbol{y} + \dot{\boldsymbol{\alpha}}_0(t)] \cdot \frac{\partial}{\partial \boldsymbol{x}}\,\delta(\boldsymbol{x} - \boldsymbol{y}) + \tfrac{1}{2}\dot{\boldsymbol{\sigma}}_0(t) : \frac{\partial^2}{\partial \boldsymbol{x}\,\partial \boldsymbol{x}}\,\delta(\boldsymbol{x} - \boldsymbol{y}), \tag{2.2.31}$$

where

$$\dot{\boldsymbol{\rho}}_0(t) = \frac{\mathrm{d}}{\mathrm{d}s}\,\boldsymbol{\rho}(s, t)|_{s=t^+}, \qquad \dot{\boldsymbol{\alpha}}_0(t) = \frac{\mathrm{d}}{\mathrm{d}s}\,\boldsymbol{\alpha}(s, t)|_{s=t^+}, \qquad \dot{\boldsymbol{\sigma}}_0 = \frac{\mathrm{d}}{\mathrm{d}s}\,\boldsymbol{\sigma}(s, t)|_{s=t^+}. \tag{2.2.32}$$

From (1.3.43) and (1.3.49) it follows that

$$\dot{\sigma}_0(t) = \dot{\sigma}_0^{\dagger}(t) \text{ non-negative definite.} \tag{2.2.33}$$

The kernel (2.2.31) is equivalent to the Fokker–Planck-operator

$$\Gamma(t) = -\frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{v}(\boldsymbol{x}t) + \frac{\partial^2}{\partial \boldsymbol{x}\,\partial \boldsymbol{x}} : \mathbf{D}(t) \tag{2.2.34}$$

$$\Gamma^{\dagger}(t) = \boldsymbol{v}(\boldsymbol{x}t) \cdot \frac{\partial}{\partial \boldsymbol{x}} + \mathbf{D}(t) : \frac{\partial^2}{\partial \boldsymbol{x}\,\partial \boldsymbol{x}} \tag{2.2.35}$$

with linear drift vector

$$\boldsymbol{v}(\boldsymbol{x}t) = \dot{\boldsymbol{\rho}}_0(t) \cdot \boldsymbol{x} + \dot{\boldsymbol{\alpha}}_0(t) \tag{2.2.36}$$

and state-independent diffusion tensor

$$\mathbf{D}(t) = \tfrac{1}{2}\dot{\boldsymbol{\sigma}}_0(t). \tag{2.2.37}$$

For the time evolution of the vector of mean values $\boldsymbol{a}(t)$ and the equal-time covariance matrix $\mathbf{s}(t)$, one obtains from (1.3.44, 46) the differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{a}(t) = \dot{\boldsymbol{\alpha}}_0(t) + \dot{\boldsymbol{\rho}}_0(t) \cdot \boldsymbol{a}(t) \tag{2.2.38}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{s}(t) = \dot{\boldsymbol{\sigma}}_0(t) + \dot{\boldsymbol{\rho}}_0(t) \cdot \mathbf{s}(t) + \mathbf{s}(t) \cdot \dot{\boldsymbol{\rho}}_0^{\dagger}(t)\,. \tag{2.2.39}$$

For a Markov process, $\boldsymbol{\rho}_0(t)$, $\boldsymbol{\alpha}_0(t)$ and $\boldsymbol{\sigma}_0(t)$ determine the time evolution of the quantities $\boldsymbol{\rho}(t, t_1)$, $\boldsymbol{\alpha}(t, t_1)$ and $\boldsymbol{\sigma}(t, t_1)$. From the Markov conditions (1.3.50–52), one obtains the differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\rho}(t, t_1) = \dot{\boldsymbol{\rho}}_0(t) \cdot \boldsymbol{\rho}(t, t_1) \tag{2.2.40}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\alpha}(t, t_1) = \dot{\boldsymbol{\alpha}}_0(t) + \dot{\boldsymbol{\rho}}_0(t) \cdot \boldsymbol{\alpha}(t, t_1) \tag{2.2.41}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\sigma}(t, t_1) = \dot{\boldsymbol{\sigma}}_0(t) + \dot{\boldsymbol{\rho}}_0(t) \cdot \boldsymbol{\sigma}(t, t_1) + \boldsymbol{\sigma}(t, t_1) \cdot \dot{\boldsymbol{\rho}}_0^{\dagger}(t) \tag{2.2.42}$$

which have the solutions

$$\boldsymbol{\rho}(t, t_1) = \mathscr{T} \exp\left[\int_{t_1}^{t} \dot{\boldsymbol{\rho}}_0(s)\,\mathrm{d}s\right] \tag{2.2.43}$$

$$\boldsymbol{\alpha}(t, t_1) = \int_{t_1}^{t} \boldsymbol{\rho}(t, s) \cdot \dot{\boldsymbol{\alpha}}_0(s)\,\mathrm{d}s \tag{2.2.44}$$

$$\boldsymbol{\sigma}(t, t_1) = \int_{t_1}^{t} \boldsymbol{\rho}(t, s) \cdot \dot{\boldsymbol{\sigma}}_0(s) \cdot \boldsymbol{\rho}^{\dagger}(t, s)\,\mathrm{d}s\,, \tag{2.2.45}$$

where $\mathscr{T}$ is the time-ordering operator.

For a time-homogeneous process, $\dot{\boldsymbol{\rho}}_0 = \text{const.}$, $\dot{\boldsymbol{\alpha}}_0 = \text{const.}$, $\dot{\boldsymbol{\sigma}}_0 = \text{const.}$, the solution (2.2.43) takes the form

$$\boldsymbol{\rho}(\tau) = \exp(\dot{\boldsymbol{\rho}}_0 \tau)\,. \tag{2.2.46}$$

It should be noted that so far no condition has been introduced for the quantity $\dot{\boldsymbol{\rho}}_0$. One may have, in particular, time-homogeneous (but nonstationary) Gauss–Markov processes for which the eigenvalues of $\dot{\boldsymbol{\rho}}_0$ have positive real parts. Such processes have an application for the description of the onset of decay of an unstable state [42].

If the process is stationary, then it follows from (2.2.38, 39) that $\dot{\boldsymbol{\rho}}_0$, $\dot{\boldsymbol{\alpha}}_0$ and $\dot{\boldsymbol{\sigma}}_0$ are related by

$$\dot{\boldsymbol{\alpha}}_0 + \dot{\boldsymbol{\rho}}_0 \cdot \boldsymbol{a} = 0 \tag{2.2.47}$$

and

$$\dot{\boldsymbol{\sigma}}_0 + \dot{\boldsymbol{\rho}}_0 \cdot \mathbf{s} + \mathbf{s} \cdot \dot{\boldsymbol{\rho}}_0^{\dagger} = 0 \,. \tag{2.2.48}$$

Since by (1.1.23) and (2.2.33) both $\mathbf{s}$ and $\dot{\boldsymbol{\sigma}}_0$ are non-negative definite, the latter relation represents a strong condition for $\dot{\boldsymbol{\rho}}_0$. If both quantities are positive definite, one can show by a slight generalization of a theorem given in [43] that $\dot{\boldsymbol{\rho}}_0$ is a *stability matrix*, i.e.

all eigenvalues of $\dot{\boldsymbol{\rho}}_0$ have negative real part. (2.2.49)

Thus, any stationary Gauss–Markov process with $\mathbf{s}$ and $\dot{\boldsymbol{\sigma}}_0$ positive definite is asymptotically stable (see section 3.4). For a stationary process, the solutions of the differential Markov conditions (2.2.41, 42) can with the help of (2.2.47, 48) be written in the form

$$\boldsymbol{\alpha}(\tau) = [\mathbf{1} - \exp(\dot{\boldsymbol{\rho}}_0 \tau)] \cdot \boldsymbol{a} \tag{2.2.50}$$

$$\boldsymbol{\sigma}(\tau) = \mathbf{s} - \exp(\dot{\boldsymbol{\rho}}_0 \tau) \cdot \mathbf{s} \cdot \exp(\dot{\boldsymbol{\rho}}_0^{\dagger} \tau) \,. \tag{2.2.51}$$

For the case of the Wiener process (1.3.64, 65), one has

$$\dot{\alpha}_0 = \dot{\rho}_0 = 0 \,, \qquad \dot{\sigma}_0 = 2D = 1 \,, \tag{2.2.52}$$

which yields the master operator

$$\Gamma = \tfrac{1}{2} \partial^2 / \partial x^2 \,. \tag{2.2.53}$$

The time derivative $\zeta(t) = \dot{x}(t)$ of the Wiener process is the stationary Gaussian δ-correlated process ("white noise") with

$$\langle \zeta(t) \rangle = 0 \tag{2.2.54a}$$

$$\langle \zeta(t)\, \zeta(s) \rangle = \delta(t - s) \,. \tag{2.2.54b}$$

2.3. *Properties of the master operator. Kramers–Moyal expansion*

Properties of the propagator set $R(t|s)$ and of the master operator $\Gamma(t)$ depend on the nature of the sample functions of the process. Three distinct cases are of importance: Purely deterministic drift represented by a first-order differential operator $\Gamma(t)$ (e.g. Liouville operator), diffusion processes with sample functions which are almost everywhere continuous but almost nowhere differentiable, represented by a second-order differential operator $\Gamma(t)$ (Fokker–Planck operator), and jump processes with piecewise constant sample functions, represented by an integral operator $\Gamma(t)$ with kernel $\Gamma(x, y; t)$. (All processes considered are assumed to be stochastically continuous and stochastically differentiable in the sense of eqs. (1.3.10) and (2.2.2).) More general processes may be obtained as superpositions of these pure cases.

We start with a brief discussion of jump processes. From the significance of the conditional probability it is seen that $\Gamma(x, y; t)\,dx$ represents for $x \neq y$ the jump rate for jumps $y \to (x, x + dx)$, whereas for $x = y$ the kernel $\Gamma(x, y; t)$ contains a negative δ-function contribution representing the loss of weight of state y due to all jumps starting at y. Hence the kernel $\Gamma(x, y; t)$ can be written (see fig. 2):

$$\Gamma(x, y; t) = W(x, y; t) - \gamma(yt)\,\delta(x - y) \tag{2.3.1a}$$

$$= \gamma(yt)\,[\rho(x - y, y; t) - \delta(x - y)]\,, \tag{2.3.1b}$$

where

$$W(x, y; t) \geq 0 \tag{2.3.2}$$

is the jump rate for jumps $y \to (x, x + dx)$,

$$\gamma(yt) = \int W(x, y; t)\,dx \tag{2.3.3}$$

is the total jump rate for jumps starting at y, and

$$\rho(r, y; t) = \frac{1}{\gamma(yt)}\,W(y + r, y; t) \tag{2.3.4}$$

is the probability distribution for the jump width r for jumps starting at y.

It is easily seen that $\Gamma(x, y; t)$ satisfies the condition for conservation of the normalization of the probability

$$\int \Gamma(x, y; t)dx = 0\,. \tag{2.3.5}$$

By using eqs. (2.2.12), (2.3.1a) and (2.3.3), we obtain the master equation in the usual form

$$\frac{\partial p(xt)}{\partial t} = \int [W(x, y; t)\,p(yt) - W(y, x; t)\,p(xt)]\,dy\,. \tag{2.3.6}$$

It may be expected that one can pass from a jump process to a process with continuous sample functions in the limit of jump width $\to 0$, jump rate $\to \infty$. We study this limit by a simple scaling procedure. We regard the transition rate $W(x, y; y)$ as a function $P(r, y; t)$ of jump width $r = x - y$ and starting point y, and consider a two-parameter family of jump processes, each with the same functional form of P, but differing in average jump rate ν and average jump width l. Taking the normalization required by eq. (2.3.3) into account, we have

$$P(r, y; t) = \frac{\nu}{l}\,\bar{P}\left(\frac{1}{l}\,r, y; t\right), \tag{2.3.7}$$

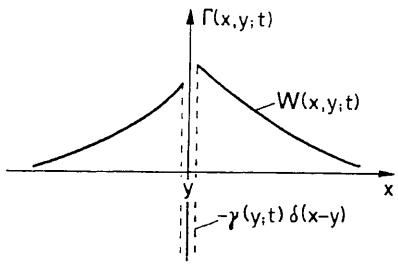

Fig. 2. Structure of the kernel $\Gamma(x, y; t) = W(x, y; t) - \gamma(y; t)\,\delta(x - y)$ of the master operator.

where the function $\tilde{P}$ is independent of ν and l. With $\boldsymbol{u} = \boldsymbol{r}/l$ as integration variable, the master equation (2.3.6) takes the form

$$\frac{\partial p(\boldsymbol{x}t)}{\partial t} = \nu \int [\tilde{P}(\boldsymbol{u}, \boldsymbol{x} - l\boldsymbol{u}; t)\, p(\boldsymbol{x} - l\boldsymbol{u}, t) - \tilde{P}(\boldsymbol{u}, \boldsymbol{x}; t)\, p(\boldsymbol{x}t)]\, \mathrm{d}u . \tag{2.3.8}$$

Taylor expansion with respect to the average jump width l up to second order yields the *Fokker–Planck* equation

$$\frac{\partial p(\boldsymbol{x}t)}{\partial t} = -\frac{\partial}{\partial \boldsymbol{x}} \cdot [\boldsymbol{v}(\boldsymbol{x}t)\, p(\boldsymbol{x}t)] + \frac{\partial^2}{\partial \boldsymbol{x}\, \partial \boldsymbol{x}} : [\mathbf{D}(\boldsymbol{x}t)\, p(\boldsymbol{x}t)] \tag{2.3.9}$$

with a drift vector

$$\boldsymbol{v}(\boldsymbol{x}t) = \nu l \int \boldsymbol{u}\, \tilde{P}(\boldsymbol{u}, \boldsymbol{x}; t)\, \mathrm{d}u = \int \boldsymbol{r}\, W(\boldsymbol{x} + \boldsymbol{r}, \boldsymbol{x}; t)\, \mathrm{d}r \equiv \nu l \bar{\boldsymbol{u}} \tag{2.3.10}$$

and a non-negative definite diffusion tensor

$$\mathbf{D}(\boldsymbol{x}t) = \tfrac{1}{2}\nu l^2 \int \boldsymbol{u}\boldsymbol{u}\, \tilde{\boldsymbol{P}}(\boldsymbol{u}, \boldsymbol{x}; t)\, \mathrm{d}u = \tfrac{1}{2} \int \boldsymbol{r}\boldsymbol{r}\, W(\boldsymbol{x} + \boldsymbol{r}, \boldsymbol{x}; t)\, \mathrm{d}r \equiv \tfrac{1}{2}\nu l^2 \overline{\boldsymbol{u}\boldsymbol{u}} . \tag{2.3.11}$$

Thus, jumps with $\bar{u} \neq 0$ of rate $\nu \propto 1/l$ give rise to drift, and jumps with $\bar{u} = 0$ but $\overline{uu} \neq 0$ of rate $\nu \propto 1/l^2$ give rise to diffusion. In order to obtain the Fokker–Planck equation (2.3.9) with both drift and diffusion, both types of jump processes have to be present.

This scaling procedure gives of course no information on the convergence properties of the Taylor expansion. It is important to note, however, that there exists no scaling yielding a truncation of the Taylor expansion at a finite $n > 2$: A scaling $\nu \propto l^{-n}$ leads for asymmetric jumps to a divergence $v \propto l^{-n+1}$ of the drift velocity, and for symmetric jumps to a divergence $D \propto l^{-n+2}$ of the diffusion coefficient.

On the other hand, the formal Taylor expansion yields a representation of the integral operator $\Gamma(t)$ as an infinite-order differential operator. Writing the kernel of $\Gamma(t)$ as

$$\Gamma(\boldsymbol{x}, \boldsymbol{y}; t) = \int \Gamma(\boldsymbol{z}, \boldsymbol{y}; t)\, \delta(\boldsymbol{z} - \boldsymbol{x})\, \mathrm{d}z \tag{2.3.12}$$

and formally expanding the δ-function at $\boldsymbol{z} = \boldsymbol{y}$ in powers of $\boldsymbol{z} - \boldsymbol{y}$ yields the representation

$$\Gamma(\boldsymbol{x}, \boldsymbol{y}; t) = \sum_{n=1}^{\infty} \frac{1}{n!} \mathbf{A}_n(\boldsymbol{y}t) \odot \left(\frac{\partial}{\partial \boldsymbol{y}}\right)^{[n]} \delta(\boldsymbol{y} - \boldsymbol{x}) . \tag{2.3.13}$$

Here, $\boldsymbol{v}^{[n]}$ denotes the n-fold dyadic product of the vector $\boldsymbol{v}$, $\mathbf{A}_n$ is the $n \times n$ matrix

$$\mathbf{A}_n(\boldsymbol{y}t) = \int (\boldsymbol{z} - \boldsymbol{y})^{[n]}\, \Gamma(\boldsymbol{z}, \boldsymbol{y}; t)\, \mathrm{d}z \tag{2.3.14}$$

assumed to exist for all $n = 1, 2, \ldots$, and the notation $L \odot M$ stands for the n-fold contraction of two

$n \times n$ matrices L and M (note that $A_0 = 0$ on account of (2.3 With (2.3.13) one obtains for the master equation by partial integration the *Kramers–Moyal expansion* [42, 44]

$$\frac{\partial p(xt)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \left(\frac{\partial}{\partial x}\right)^{[n]} \odot [\mathbf{A}_n(xt)\, p(xt)]\,. \tag{2.3.15}$$

An alternative representation is obtained from

$$\Gamma(x, y; t) = \int \Gamma(x, z; t)\, \delta(z - y)\, \mathrm{d}z \tag{2.3.16}$$

yielding

$$\Gamma(x, y; t) = \sum_{n=0}^{\infty} \frac{1}{n!} \mathbf{a}_n(xt) \odot \left(\frac{\partial}{\partial x}\right)^{[n]} \delta(x - y) \tag{2.3.17}$$

with

$$\mathbf{a}_n(xt) = \int (z - x)^{[n]}\, \Gamma(x, z; t)\, \mathrm{d}z \tag{2.3.18}$$

which is assumed to exist for all $n = 0, 1, 2, \ldots$. This gives rise to the expansion

$$\frac{\partial p(xt)}{\partial t} = \sum_{n=0}^{\infty} \frac{1}{n!} \mathbf{a}_n(xt) \odot \left(\frac{\partial}{\partial x}\right)^{[n]} p(xt) \tag{2.3.19}$$

which in contrast to the Kramers–Moyal expansion starts with $n = 0$. The sets of expansion coefficients $\mathbf{A}_n(xt)$ and $\mathbf{a}_n(xt)$ are related by

$$\mathbf{A}_n(xt) = \sum_{l=0}^{\infty} \frac{(-1)^{n+l}}{l!} \left(\frac{\partial}{\partial x}\right)^{[l]} \odot \mathbf{a}_{n+l}(xt) \tag{2.3.20}$$

$$\mathbf{a}_n(xt) = \sum_{l=0}^{\infty} \frac{(-1)^{n+l}}{l!} \left(\frac{\partial}{\partial x}\right)^{[l]} \odot \mathbf{A}_{n+l}(xt)\,. \tag{2.3.21}$$

The alternative expansion (2.3.19) should not be confused with the backward equation of the Kramers–Moyal expansion (2.3.15). The backward equation can be written in the alternative forms

$$\frac{\partial f(xt)}{\partial t} = \sum_{n=1}^{\infty} \frac{1}{n!} \mathbf{A}_n(xt) \odot \left(\frac{\partial}{\partial x}\right)^{[n]} f(xt) \tag{2.3.22}$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(\frac{\partial}{\partial x}\right)^{[n]} \odot [\mathbf{a}_n(xt)\, f(xt)]\,. \tag{2.3.23}$$

It is important to note that truncation of the series (2.3.15) at any order higher than the second will lead to inconsistencies, as was already concluded from the above scaling argument. This is a

consequence of the truncation lemma of Pawula [45–47]: If it is assumed that $\mathbf{A}_n$ (or $\mathbf{a}_n$, respectivly) vanishes identically for some $n_0 \geq 3$, then it follows that the $\mathbf{A}_n$ (or $\mathbf{a}_n$) have to vanish identically for all $n \geq 3$. The only consistent finite-order differential master equation is thus the Fokker–Planck equation with

$$\boldsymbol{v}(\boldsymbol{x}t) = \boldsymbol{A}_1(\boldsymbol{x}t), \qquad \mathbf{D}(\boldsymbol{x}t) = \tfrac{1}{2}\mathbf{A}_2(\boldsymbol{x}t)\,. \tag{2.3.24}$$

The problem of the convergence of a sequence of processes $\boldsymbol{x}_\varepsilon(t)$ with decreasing fluctuation strength ε, and the extent to which such processes may be approximated by diffusion processes when ε is sufficiently small attracts presently a great deal of interest [48–54]. This problem is quite subtle, and a definite solution is not yet available.

2.3.E1. Time evolution of the process with independent increments

We consider as an example the time-homogeneous Markov process with independent increments introduced in section 1.3.E3. From (1.3.67) and (2.2.2) it is seen that the kernel $\Gamma(\boldsymbol{x}, \boldsymbol{y}; t)$ of the master operator becomes a function of the jump width $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{y}$ only.

According to (2.3.1b) it can be written

$$\Gamma(\boldsymbol{r}) = \gamma[\rho(\boldsymbol{r}) - \delta(\boldsymbol{r})]\,, \tag{2.3.25}$$

where γ is the jump frequency and $\rho(\boldsymbol{r})$ is the probability distribution for the jump width $\boldsymbol{r}$. The forward equation (2.2.4)

$$\frac{\partial}{\partial t} R(\boldsymbol{x}, t) = \gamma\left[\int \rho(\boldsymbol{x} - \boldsymbol{y}) R(\boldsymbol{y}, t)\, \mathrm{d}\boldsymbol{y} - R(\boldsymbol{x}, t)\right] \tag{2.3.26}$$

can be solved in closed form by Fourier transformation. In terms of the Fourier transforms $R(\boldsymbol{q}, t)$ and $\rho(\boldsymbol{q})$ of $R(\boldsymbol{x}, t)$ and $\rho(\boldsymbol{r})$, respectively, the forward equation is

$$\frac{\partial}{\partial t} R(\boldsymbol{q}, t) = \gamma[\rho(\boldsymbol{q}) - 1]\, R(\boldsymbol{q}, t) \tag{2.3.27}$$

which has the solution (note $R(\boldsymbol{q}, 0) = 1$)

$$R(\boldsymbol{q}, t) = \exp\{\gamma[\rho(\boldsymbol{q}) - 1]t\}\,. \tag{2.3.28}$$

Taylor expansion in terms of $\rho(q)$ and retransformation yields the expression

$$\begin{aligned} R(\boldsymbol{x}, t) &= \sum_{k=0}^{\infty} P(k, t) \int \cdots \int \delta\Big(\boldsymbol{x} - \sum_{i=1}^{k} \boldsymbol{r}_i\Big)\rho(\boldsymbol{r}_1) \cdots \rho(\boldsymbol{r}_k)\, \mathrm{d}^k r \\ &= \sum_{k=0}^{\infty} P(k, t) \Big\langle \delta\Big(\boldsymbol{x} - \sum_{i=1}^{k} \boldsymbol{r}_i\Big)\Big\rangle_\rho \end{aligned} \tag{2.3.29}$$

which has the obvious interpretation of the probability distribution for distance $\boldsymbol{x}$ to be reached in k

jumps with widths $r_1, \ldots r_k$, folded with the Poissonian probability

$$P(k, t) = (\gamma t)^k \exp(-\gamma t)/k! \tag{2.3.30}$$

for k jumps to occur during time t.

With the help of (2.3.29) it is straightforward to calculate conditional moments $\langle (x(t))^{[n]} | 0 \rangle$ which are equal to the moments $\langle (\Delta x(t))^{[n]} \rangle$ of the increments $\Delta x(t) = x(t+s) - x(s)$. Time correlations can be calculated recursively by making use of the independence of the increments. For an ordered set $\{t_2, t_1, s_n, \ldots s_1\} \equiv \{t_2, t_1, S\}$ of time instants one has for any function $g(S)$

$$\langle (x(t_2) - x(t_1))^{[n]} \, g(YS) \rangle = \langle (x(t_2 - t_1))^{[n]} \, | 0 \rangle \langle g(YS) \rangle \, . \tag{2.3.31}$$

For a one-dimensional process starting at $t = 0$ with $x = 0$ one finds the moments

$$\langle x(t) \rangle = \gamma t \langle r \rangle_\rho \tag{2.3.32a}$$

$$\langle x^2(t) \rangle = \gamma t \langle r^2 \rangle_\rho + (\gamma t)^2 \langle r \rangle_\rho^2 \tag{2.3.32b}$$

$$\langle x^3(t) \rangle = \gamma t \langle r^3 \rangle_\rho + 3(\gamma t)^2 \langle r^2 \rangle_\rho \langle r \rangle_\rho + (\gamma t)^3 \langle r \rangle_\rho^3 \tag{2.3.32c}$$

$$\langle x^4(t) \rangle = \gamma t \langle r^4 \rangle_\rho + (\gamma t)^2 [4 \langle r^3 \rangle_\rho \langle r \rangle_\rho + 3 \langle r^2 \rangle_\rho^2] + 6(\gamma t)^3 \langle r^2 \rangle_\rho \langle r \rangle_\rho^2 + \langle \gamma t \rangle^4 \langle r \rangle_\rho^4 \, . \tag{2.3.32d}$$

Thus, for asymmetric jumps with $\langle r \rangle_\rho \neq 0$,

$$\langle x(t) \rangle = \gamma t \langle r \rangle_\rho \tag{2.3.33}$$

$$\langle x^2(t) \rangle - \langle x(t) \rangle^2 = \gamma t \langle r^2 \rangle_\rho \tag{2.3.34}$$

one finds in the drift limit

$$\gamma \to \infty, \qquad \langle r \rangle_\rho \to 0, \qquad \langle r^2 \rangle_\rho \to 0, \qquad \gamma \langle r \rangle_\rho \to v, \qquad \gamma \langle r^2 \rangle_\rho \to 0 \tag{2.3.35}$$

a constant drift with vanishing variance, i.e.

$$x(t) = vt \text{ with probability } 1 \, . \tag{2.3.36}$$

For jumps with $\langle r \rangle_\rho = 0$, one finds in the diffusion limit

$$\gamma \to \infty, \qquad \langle r^2 \rangle_\rho \to 0, \qquad \langle r^4 \rangle_\rho \to 0, \qquad \gamma \langle r^2 \rangle_\rho \to 2D, \qquad \gamma \langle r^4 \rangle_\rho \to 0 \tag{2.3.37}$$

for $D = \frac{1}{2}$ the Wiener process (see (1.3.64, 65) and (2.2.52, 53)) with

$$\langle x(t) \, x(s) \rangle = \min(s, t) \tag{2.3.38}$$

$$\langle x^4(t) \rangle = 3t^2 \, . \tag{2.3.39}$$

Thus, $x^2(t)$ has nonvanishing variance. However, it is interesting to study also the integral $\int (\mathrm{d}x(t))^2$

defined as the limit of the sum of the squares of the increments $\Delta x_i = x(t_i) - x(t_i - 1)$ for a partition $\{t_0, t_1, \ldots t_N = t\}$ of the interval (t_0, t). One finds

$$\left\langle \sum_i (\Delta x_i)^2 \right\rangle = \gamma \langle r^2 \rangle_\rho \, (t - t_0) \tag{2.3.40}$$

$$\left\langle \left[\sum_i (\Delta x_i)^2 \right]^2 \right\rangle - \left\langle \sum_i (\Delta x_i)^2 \right\rangle^2 = \gamma \langle r^4 \rangle_\rho \, (t - t_0) + 2\gamma^2 \langle r^2 \rangle_\rho^2 \sum_i (t_i - t_{i-1})^2 . \tag{2.3.41}$$

By passing to the Riemann limit $N \to \infty$, $\max(t_i - t_{i-1}) \to 0$, the last term vanishes $\sim 1/N$. Thus, in the diffusion limit (2.3.37), the variance vanishes, and one obtains for the Wiener process

$$\int_{t_0}^{t} [\mathrm{d}x(t)]^2 = t - t_0 \text{ with probability 1.} \tag{2.3.42}$$

It should be noted that the integration over a nonzero interval is essential: $\int_{\Delta t} [\mathrm{d}x(t)]^2$ cannot be approximated by $[x(t + \Delta t) - x(t)]^2$ but must be considered as the limit of $\Sigma [x(t_i) - x(t_{i-1})]^2$ where the t_i form a partition of the interval Δt. In fact, $[x(t + \Delta t) - x(t)]^2$ has nonvanishing variance $2(\Delta t)^2$. It is the destructive interference of the statistically independent fluctuations of the terms in the sum which causes the fluctuations of the sum to vanish in the limit.

2.4. The Fokker–Planck process; stochastic differential equations

Stochastic differential equations have attracted principal interest in the context of phenomenological modelling of stochastic processes. On the deterministic level, the time evolution of the system is usually assumed to be determined by an equation of motion of the form

$$\dot{\boldsymbol{a}}(t) = \boldsymbol{u}(\boldsymbol{a}(t), t) \tag{2.4.1}$$

giving the rate of change of state $\boldsymbol{a}(t)$ as a generally nonlinear vectorial state function $\boldsymbol{u}(t)$ (deterministic drift) at the same time, independent of previous history. Fluctuations will change the deterministic process $\boldsymbol{a}(t)$ into a stochastic process $\boldsymbol{x}(t)$. They are taken into account by coupling (generally state-dependent) *stochastic forces* $\boldsymbol{X}(\boldsymbol{x}(t), t)$ into the equation of motion, giving rise to the *Langevin equation*

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{v}(\boldsymbol{x}(t), t) + \boldsymbol{X}(\boldsymbol{x}(t), t) , \tag{2.4.2}$$

which has to be supplemented by specifying the stochastic process $\boldsymbol{X}(\boldsymbol{x}, t)$.

The microscopic basis for this ansatz is related to the notion discussed in section 2.1: It is assumed that the variables of the system separate into two classes: One class of slowly varying macroscopic variables $\boldsymbol{x}(t)$ the motion of which is determined by the drift vector $\boldsymbol{v}(\boldsymbol{x}t)$, and the rest of microscopic variables varying on a much shorter time scale and giving rise to random perturbations $\boldsymbol{X}(\boldsymbol{x}, t)$ of the macroscopic motion [3, 13, 55]. – Such *stochastic differential equations* are studied extensively in the mathematical literature [56–66].

It is important to note that the drift $\boldsymbol{u}(at)$ describing the motion of the average $\boldsymbol{a}(t) = \langle \boldsymbol{x}(t) \rangle$ in a deterministic equation of the form (2.4.1) is in general not identical with the drift $\boldsymbol{v}(\boldsymbol{x}t)$ in (2.4.2) but contains nonlinear effects of the fluctuations. This is one of the problems of any phenomenological modelling: The deterministic equation does not even determine the drift term uniquely.

In the following, we confine ourselves to processes $\boldsymbol{x}(t)$ which can be approximated by Markov processes with continuous sample functions (*Fokker–Planck processes*). According to the discussion in the previous subsection, such a process may – apart from a drift – be considered as the limit of a symmetric jump process with jump frequency $\nu \to \infty$ and jump width $l \to 0$ such that $\nu l^2 = \text{const}$. Therefore, the noise contribution $\boldsymbol{X}(\boldsymbol{x}t)$ to the time derivative $\dot{\boldsymbol{x}}(t)$ consists of impulses with $X = \pm\infty$ represented by δ-functions of weight $\propto \pm l$ occurring with frequency $\nu \propto 1/l^2$ (we assume that asymmetric jumps with $\nu \propto 1/l$ are absorbed into the drift vector $\boldsymbol{v}(\boldsymbol{x}t)$). Sample functions of such a process do clearly not exist in the normal sense in the limit $\nu \to \infty$, $l \to 0$, $\nu l^2 = \text{const}$. [56–63]. It is therefore more appropriate to write the stochastic differential equation in the form of a difference equation

$$\mathrm{d}\boldsymbol{x}(t) = \boldsymbol{v}(\boldsymbol{x}(t), t)\,\mathrm{d}t + \mathrm{d}\boldsymbol{Z}(\boldsymbol{x}(t), t) \tag{2.4.3}$$

where integration over a physically small but mathematically nonzero time increment $\mathrm{d}t$ is implied.

In order for the process $\boldsymbol{x}(t)$ to be a continuous Markov process, the diffusion-induced increment $\mathrm{d}\boldsymbol{Z}(\boldsymbol{x}t)$ may be represented in terms of the increment $\mathrm{d}\boldsymbol{w}(t)$ of an m-component vectorial Wiener process satisfying (see (2.3.38, 42))

$$\langle \boldsymbol{w}(s)\,\boldsymbol{w}(t) \rangle = \mathbf{1} \min(s, t) \tag{2.4.4}$$

$$\mathrm{d}\boldsymbol{w}(t)\,\mathrm{d}\boldsymbol{w}(t) = \mathbf{1}\,\mathrm{d}t \text{ with probability 1} \tag{2.4.5}$$

in the form

$$\mathrm{d}\boldsymbol{Z}(\boldsymbol{x}(t), t) = \mathbf{b}(\boldsymbol{x}(t), t) \cdot \mathrm{d}\boldsymbol{w}(t)\,. \tag{2.4.6}$$

Here, we have introduced an m-dimensional linear state space Ω with states $\boldsymbol{w} \in \Omega$, and $\mathbf{b}(\boldsymbol{x}t)$ which is assumed smooth in both arguments represents a mapping of Ω to the vectors of Σ in $\boldsymbol{x}$. The dimension m of Ω may be smaller than, equal to, or even larger than the dimension of Σ [56–58, 64a,b]. For a mapping $\mathbf{b}(\boldsymbol{x}t)$ which depends on the state $\boldsymbol{x}$ it has become common to refer to $\mathrm{d}\boldsymbol{Z}(\boldsymbol{x}(t), t) = \mathbf{b}(\boldsymbol{x}(t), t) \cdot \mathrm{d}\boldsymbol{w}(t)$ as "multiplicative" noise in contradistinction to state-independent "additive" noise $\mathrm{d}\boldsymbol{Z}(t) = \mathbf{b}(t) \cdot \mathrm{d}\boldsymbol{w}(t)$.

In the case of multiplicative noise, the Stieltjes integral $\mathbf{b}(\boldsymbol{x}(t), t) \cdot \mathrm{d}\boldsymbol{w}(t)$ in (2.4.6) is not uniquely defined, because the sample functions of the Wiener process $\boldsymbol{w}(t)$ and therefore also of the process $\boldsymbol{x}(t)$ under consideration are not of bounded variation. *Stochastic integrals* of the form $\int Y(t)\,\mathrm{d}y(t)$ where both $Y(t)$ and $y(t)$ are processes of unbounded variation have to be defined by specifying the exact form of the terms in the Riemann approximations to the integral [56–63]. The two most important forms are the following:

Ito:

$$\int Y(t) \bullet \mathrm{d}y(t) = \lim \sum_i Y(t_{i-1})\,(y(t_i) - y(t_{i-1})) \tag{2.4.7}$$

Stratonovich:

$$\int Y(t) \bigcirc \mathrm{d}y(t) = \lim \sum_i \tfrac{1}{2}(Y(t_i) + Y(t_{i-1}))\,(y(t_i) - y(t_{i-1})) \tag{2.4.8}$$

distinguished by the multiplication symbol ● and ○, respectively. Whereas the Ito form is mathematically more convenient because $Y(t)$ is statistically independent of the increment of $y(t)$, the Stratonovich form follows more familiar rules of calculation and shows simpler transformation behaviour. The two forms are related by

$$\int Y(t) \bigcirc \mathrm{d}y(t) = \int Y(t) \bullet \mathrm{d}y(t) + \tfrac{1}{2} \int \mathrm{d}Y(t)\,\mathrm{d}y(t) \tag{2.4.9}$$

where the last term may be interpreted in either sense.

By observing that with probability 1

$$\begin{aligned} \mathrm{d}\boldsymbol{x}(t)\,\mathrm{d}\boldsymbol{w}(t) &= \mathbf{b}(\boldsymbol{x}(t), t)\,\mathrm{d}t \\ \mathrm{d}\boldsymbol{x}(t)\,\mathrm{d}\boldsymbol{x}(t) &= \mathbf{b}(\boldsymbol{x}(t), t) \cdot \mathbf{b}^{\dagger}(\boldsymbol{x}(t), t)\,\mathrm{d}t \end{aligned} \tag{2.4.10}$$

one obtains from (2.4.9) with $Y(t) = \mathbf{b}(\boldsymbol{x}(t), t)$ and $y(t) = \boldsymbol{w}(t)$ for the stochastic forces (2.4.6)

$$\mathbf{b}(x(t), t) \bigcirc \mathrm{d}\boldsymbol{w}(t) = \mathbf{b}(x(t), t) \bullet \mathrm{d}\boldsymbol{w}(t) + \boldsymbol{v}^{\mathrm{f}}(\boldsymbol{x}(t), t)\,\mathrm{d}t \tag{2.4.11}$$

where $\boldsymbol{v}^{\mathrm{f}}(\boldsymbol{x}t)$ is a *fluctuation-induced drift* term ("spurious drift") defined by

$$v_i^{\mathrm{f}} = \tfrac{1}{2} \sum_{j\alpha} b_{j\alpha}(\partial b_{i\alpha}/\partial x_j)\,. \tag{2.4.12}$$

We thus have the two forms of stochastic differential equation:

Ito:

$$\mathrm{d}\boldsymbol{x}(t) = \boldsymbol{v}(\boldsymbol{x}(t), t)\,\mathrm{d}t + \mathbf{b}(\boldsymbol{x}(t), t) \bullet \mathrm{d}\boldsymbol{w}(t)\,, \tag{2.4.13}$$

Stratonovich:

$$\mathrm{d}\boldsymbol{x}(t) = \boldsymbol{u}(x(t), t)\,\mathrm{d}t + \mathbf{b}(\boldsymbol{x}(t), t) \bigcirc \mathrm{d}\boldsymbol{w}(t)\,, \tag{2.4.14}$$

where the Ito drift $\boldsymbol{v}(\boldsymbol{x}t)$ differs from the Stratonovich drift $\boldsymbol{u}(\boldsymbol{x}t)$ by the fluctuation-induced drift (2.4.12),

$$\boldsymbol{v}(\boldsymbol{x}t) = \boldsymbol{u}(\boldsymbol{x}t) + \boldsymbol{v}^{\mathrm{f}}(\boldsymbol{x}t)\,. \tag{2.4.15}$$

It is important to note, that only if (2.4.6) is interpreted in the Ito sense, show the fluctuating forces $\boldsymbol{X}(t) = \mathrm{d}\boldsymbol{Z}(\boldsymbol{x}(t), t)/\mathrm{d}t$ the properties of white (i.e. δ-correlated) noise [66] characterized by the conditional averages

$$\langle \boldsymbol{X}(t) | \boldsymbol{x}(t) = \boldsymbol{x}_t \rangle = 0 \tag{2.4.16}$$

$$\langle \boldsymbol{X}(t)\, \boldsymbol{X}(s) | \boldsymbol{x}(t) = \boldsymbol{x}_t \rangle = \mathbf{b}(\boldsymbol{x}_t, t) \cdot \mathbf{b}^{\dagger}(\boldsymbol{x}_t, t)\, \delta(t-s)\,. \tag{2.4.17}$$

Further,the forces $\boldsymbol{X}(t)$ are Gaussian only for additive noise. On the other hand, a procedure by which the diffusion process is generated as the limit of a sequence of processes with noise consisting of continuous sample functions of bounded variation leads directly to the Stratonovich form (2.4.14) of the stochastic differential equation [65].

The connection between the stochastic differential equation and the Fokker–Planck equation is established most directly by calculating the rate of change of the average $\langle f(t) \rangle$ of an arbitrary state function $f(\boldsymbol{x}(t))$ and comparing the result with (2.2.16). Making use of the statistical independence of the increments in the Ito form (2.4.13), one obtains by observing (2.4.10)

$$\Gamma^{\dagger}(t) = \boldsymbol{v}(\boldsymbol{x}(t), t) \cdot \frac{\partial}{\partial \boldsymbol{x}} + \tfrac{1}{2}[\mathbf{b}(\boldsymbol{x}(t), t) \cdot \mathbf{b}^{\dagger}(\boldsymbol{x}(t), t)] : \frac{\partial^2}{\partial \boldsymbol{x}\, \partial \boldsymbol{x}} \tag{2.4.18a}$$

which is the transpose of the *Fokker–Planck operator*

$$\Gamma(t) = -\frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{v}(\boldsymbol{x}(t), t) + \tfrac{1}{2} \frac{\partial^2}{\partial \boldsymbol{x}\, \partial \boldsymbol{x}} : [\mathbf{b}(\boldsymbol{x}(t),\ t) \cdot \mathbf{b}^{\dagger}(\boldsymbol{x}(t), t)]\,. \tag{2.4.18b}$$

The stochastic differential equation (2.4.13, 14) is thus equivalent to a Fokker–Planck equation (2.3.9) with a drift vector given by the Ito drift, and a non-negative definite diffusion given by

$$\mathbf{D}(\boldsymbol{x}(t), t) = \tfrac{1}{2}\mathbf{b}(\boldsymbol{x}(t), t) \cdot \mathbf{b}^{\dagger}(\boldsymbol{x}(t), t)\,. \tag{2.4.19}$$

We observe that the fluctuation matrix $\mathbf{b}(\boldsymbol{x}t)$ and therefore also the fluctuation-induced drift $\boldsymbol{v}^{\mathrm{f}}(\boldsymbol{x}t)$ are not uniquely determined by the diffusion tensor $\mathbf{D}(\boldsymbol{x}t)$. Thus, a whole set of stochastic differential equations is equivalent to a single Fokker–Planck equation. A detailed discussion of the relationship between fluctuation-induced drift and diffusion tensor is given in [64a, b].

Historically, diffusion processes were introduced by requiring the conditional probability to satisfy the following set of conditions for all $\delta > 0$ [40, 41]:

$$\int_{|\boldsymbol{\xi}| \geq \delta} R(\boldsymbol{x} + \boldsymbol{\xi},\, t + \tau | \boldsymbol{x}t)\, \mathrm{d}\boldsymbol{\xi} = \mathrm{o}(\tau) \tag{2.4.20}$$

$$\int_{|\boldsymbol{\xi}| \leq \delta} \boldsymbol{\xi}\, R(\boldsymbol{x} + \boldsymbol{\xi},\, t + \tau | \boldsymbol{x}t)\, \mathrm{d}\boldsymbol{\xi} = \tau \boldsymbol{v}(\boldsymbol{x}t) + \mathrm{o}(\tau) \tag{2.4.21}$$

$$\tfrac{1}{2} \int_{|\boldsymbol{\xi}| \leq \delta} \boldsymbol{\xi}\boldsymbol{\xi}\, R(\boldsymbol{x} + \boldsymbol{\xi},\, t + \tau | \boldsymbol{x}t)\, \mathrm{d}\boldsymbol{\xi} = \tau \mathbf{D}(\boldsymbol{x}t) + \mathrm{o}(\tau)\,. \tag{2.4.22}$$

Condition (2.4.20) guarantees the continuity of the sample functions whereas (2.4.21) and (2.4.22) which are reminiscent of (2.3.10) and (2.3.11) define the drift vector and the diffusion tensor. It should be noted that the existence of the first and second moments is not explicitly required.

We close this subsection with a brief outline of the transformation behaviour of stochastic differential

equations under general nonlinear coordinate transformations $\bar{x}^i = \bar{x}^i(x)$ in state space Σ, which will in general not be a Euclidean space but may be any curved manifold. We assume that in a given appropriately chosen set of coordinates the system is described by the stochastic differential equation (2.4.13, 14). For the transformation of the increment $dx^i(t)$ one finds by using (2.4.9, 10)

$$d\bar{x}^i(t) = \frac{\partial \bar{x}^i}{\partial x^j} \bullet dx^j(t) + \frac{1}{2} \frac{\partial^2 \bar{x}_i}{\partial x^j \partial x^k} dx^j(t)\, dx^k(t) \tag{2.4.23}$$

$$= \frac{\partial \bar{x}^i}{\partial x^j} \circ dx^j(t) .$$

(Here and in the following, summation over repeated indices is implied.) Application of $\partial \bar{x}^i / \partial x^j \circ$ to both sides of the Stratonovich equation (2.4.14) shows that this equation written out in components is already in covariant form, and that u^i and b^i_α transform contravariant (the latter with respect to index i; index α is irrelevant because the noise space Ω is left unchanged):

$$\bar{u}^i = \frac{\partial \bar{x}^i}{\partial x^j} u^j , \qquad \bar{b}^i_\alpha = \frac{\partial \bar{x}^i}{\partial x^j} b^j_\alpha , \qquad \text{i.e. } \bar{D}^{ij} = \frac{\partial \bar{x}^i}{\partial x^k} \frac{\partial \bar{x}^j}{\partial x^l} D^{kl} . \tag{2.4.24}$$

The Ito drift v^i, on the other hand, transforms inhomogeneously,

$$\bar{v}^i = \frac{\partial \bar{x}^i}{\partial x^j} v^j + \frac{1}{2} \frac{\partial^2 \bar{x}^i}{\partial x^j \partial x^k} b^j_\alpha b^k_\alpha = \frac{\partial \bar{x}^i}{\partial x^j} v^j + \frac{\partial^2 \bar{x}^i}{\partial x^j \partial x^k} D^{jk} . \tag{2.4.25}$$

The transposed Fokker–Planck operator $\Gamma^\dagger(t)$ given by (2.4.18a) may be expressed in invariant form [63b] as

$$\Gamma^\dagger(t) = u^i \frac{\partial}{\partial x^i} + \frac{1}{2} b^i_\alpha \frac{\partial}{\partial x^i} b^j_\alpha \frac{\partial}{\partial x^j} , \tag{2.4.26}$$

as is to be required of the generator of time evolution of scalar quantities $\langle f(t) \rangle$.

If the state space is a Riemannian manifold with positive definite metric tensor g_{ij}, the transposed Fokker–Planck operator may be written in terms of the invariant Laplace–Beltrami operator,

$$\Gamma^\dagger(t) = w^i \frac{\partial}{\partial x^i} + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \sqrt{g}\, D^{ij} \frac{\partial}{\partial x^j} \tag{2.4.27}$$

where $g = \det g_{ij}$, $D^{ij} = \frac{1}{2} b^i_\alpha b^j_\alpha$, and

$$w^i = v^i - \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^j} (\sqrt{g}\, D^{ij}) = u^i - \frac{1}{2} b^i_\alpha \left(\frac{\partial b^j_\alpha}{\partial x^j} + b^j_\alpha \frac{1}{\sqrt{g}} \frac{\partial \sqrt{g}}{\partial x^j} \right) . \tag{2.4.28}$$

If the diffusion tensor is nonsingular, its inverse may be used as metric tensor, in which case

$$g = (\det D^{ij})^{-1} . \tag{2.4.29}$$

From (2.4.27, 28) it is seen that the Fokker–Planck operator is determined by the diffusion matrix $D^{ij} = \frac{1}{2} b^{i\alpha} b^{j\alpha}$ alone, if

$$b^i_\alpha \left(\frac{\partial b^j_\alpha}{\partial x^j} + b^j_\alpha \frac{1}{\sqrt{g}} \frac{\partial \sqrt{g}}{\partial x^j} \right) = 0 \qquad \forall i . \tag{2.4.30}$$

An alternative kind of covariant formulation is discussed in refs. [67, 132a].

2.5. Stochastic fields

The state of an extended system is described by an n-component field $\phi(t)$ with values $\phi(rt)$. The deterministic behaviour is given by the flow

$$\dot{\phi}(t) = u[\phi(t), t] \tag{2.5.1}$$

in state space Σ which is now a functional manifold. In most applications, u is a nonlinear partial differential operator or a nonlinear integro-differential operator acting on the field $\phi(rt)$. In the presence of fluctuations, $\phi(t)$ becomes a stochastic field. In analogy to (2.4.2), the stochastic behaviour may be described by a functional Langevin equation

$$\dot{\phi}(t) = v[\phi(t), t] + \zeta[\phi(t), t] \tag{2.5.2}$$

which has to be supplemented by specifying the stochastic field $\zeta[\phi(t), t]$. Usually, one assumes without much justification that ζ can be represented by a white-noise process which is δ-correlated also in space.

Alternatively, the statistical ensemble of fields $\phi(t)$ may be described by a probability measure $p[\phi, t]$ in function space satisfying a functional master equation. For Markovian systems with realizations $\phi(t)$ which are continuous in time this takes the form of a functional Fokker–Planck equation

$$\frac{\partial p[\phi, t]}{\partial t} = -\nabla_\phi \cdot (v[\phi, t]\, p[\phi, t]) + \nabla_\phi \nabla_\phi : (D[\phi, t]\, p[\phi, t]) \tag{2.5.3a}$$

$$= -\int \mathrm{d}r' \frac{\delta}{\delta \phi(r')} (v[\phi, r't]\, p[\phi, t]) + \int\int \mathrm{d}r'\, \mathrm{d}r'' \frac{\delta^2}{\delta \phi(r')\, \delta \phi(r'')} (D[\phi, r'r''t]\, p[\phi, t]) . \tag{2.5.3b}$$

However, this representation is generally of only limited use, because the techniques of functional integration are not well developed. An exception is the case that the solution can be given in terms of a Ginzburg–Landau type functional [8, 11].

A formal device used as a poor man's substitute for functional integration is the discretization by subdivision of real space into cells [68–70], or more generally by expansion into a complete set of discrete modes $\varphi_n(r)$

$$\phi(rt) = \sum_n \phi_n(t)\, \varphi_n(r) , \tag{2.5.4}$$

combined with a truncation procedure. The stochastics of the remaining finite set $\{\phi_n(t)\}$ can then be handled by the methods described in the previous subsections.

2.6. Time evolution of non-Markov processes

In the case of non-Markov processes, the conditional probability $R(xt|ys)$, $t > s$ depends on previous history. Thus, $R(t|s)$ is not a linear operator in $\Pi(\Sigma)$ but depends in a nonlinear way on the initial distribution (fig. 3), and fails to satisfy the Chapman–Kolmogorov–Smoluchowski equation (1.3.15) which was used to derive the master equation (2.2.12) of Markov processes. It is therefore an important question whether one can construct a propagator set $G(t|s)$ for the single-event distribution

$$p(t) = G(t|s)\, p(s) \tag{2.6.1}$$

satisfying the (pseudo)-Chapman–Kolmogorov–Smoluchowski equation

$$G(t|t_1) = G(t|s)\, G(s|t_1), \qquad t \geq s \geq t_1 \tag{2.6.2}$$

and

$$G(t^+|t) = \mathbb{1}\,. \tag{2.6.3}$$

This would permit the derivation of a master equation

$$\dot{p}(t) = \Gamma(t)\, p(t) \tag{2.6.4}$$

with a stochastic operator given by

$$\Gamma(t) = \frac{\mathrm{d}}{\mathrm{d}s}\, G(s|t)|_{s=t^+}\,. \tag{2.6.5}$$

The existence of such a substitutive (pseudo)-Markov process with the same propagation behaviour of the single-event distribution has been studied by the authors [30, 33, 34, 37].

The condition (2.6.1) does not determine the propagator set $G(t|s)$ uniquely but allows the construction of many such sets, which depend in general on the initial distribution. It is important to stress that the kernels $G(xt|ys)$ of these propagator sets are in general different from the conditional

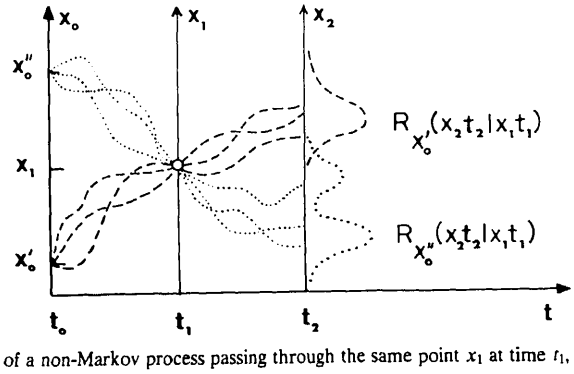

Fig. 3. Two sets of sample functions of a non-Markov process passing through the same point x_1 at time t_1, but starting at different points x_0' and x_0'' at a previous time t_0, give rise to two different conditional distributions.

probability $R(\boldsymbol{x}t|\boldsymbol{y}s)$ (they may even take on negative values), and cannot be used to calculate time correlation functions and conditional averages. There is one exception: If the coarse-grained system was prepared at time t_0 without any memory of the past, and if $R(t|t_0)$ is nonsingular for $t > t_0$, then

$$G(t|s) = R(t|t_0)\, R(s|t_0)^{-1} \tag{2.6.6}$$

is a propagator set independent of the initial distribution, and $G(t|t_0)$ coincides with $R(t|t_0)$. Therefore, $G(t|t_0)$ may be used to calculate initial correlations $C(t, t_0)$, but it is important to note that, because of the preparation procedure, these initial correlations differ from the correlations $C(t, s)$ in an aged system, even if the stationary distribution is chosen as initial condition. For the calculation of higher correlations, one has to construct propagator sets for the multivariate probabilities $p^{(n)}(t_1, \ldots t_n)$, describing an n-point pseudo-Markov process with the same propagation behaviour as $p^{(n)}$ [30].

These concepts are supported and generalised by the derivation of the evolution equation of the macrodistribution from the microdynamics of the system. The theory shows that the initial preparation of the system is of equal importance as the dynamical laws [33, 34, 37, 55]. The microdistributions consistent with a given value of the macrovariables $\boldsymbol{x}$ are characterised by the distribution $w_\pi(\boldsymbol{q}t_0|\boldsymbol{x})$ over the microstates $\boldsymbol{q}$ belonging to the value $\boldsymbol{x}$. It is found that all initial preparations given by the same $w_\pi(\boldsymbol{q}t_0|\boldsymbol{x})$ form a class π with the same macroscopic $R_\pi(t|t_0)$, independent of the initial macrodistribution $p(t_0)$, but preparations with different $w_\pi(\boldsymbol{q}t_0|\boldsymbol{x})$ give rise to different $R_\pi(t|t_0)$, and are described macroscopically as different processes. The calculation of time correlations in an aged system given by $R_\pi(t|s)$, $s > t_0$, from microdynamics requires the derivation of a propagation equation for the two-time probability which has been carried out in ref. [34]. For the special case of the stationary preparation class s, for which $w_s(qt_0|x)\ p_s(x)$ represents the stationary microdistribution of the total system, the macroscopic initial conditional probability $R_s(t|t_0)$ coincides with the time-homogeneous conditional probability of the stationary macroprocesses. Note however that the choice of an initial probability $p_0 \neq p_s$ in the stationary class will give rise to a different process-dependent aged conditional probability $R_\sigma(t|s)$.

From a practical point of view, strong deviations from Markovian behaviour can usually be traced back to the coarse-graining over a slow variable. In such cases, a less coarse-grained description including such variables in the set of macrovariables will yield a stochastic process which may be approximated more closely by a Markov process. In this context, a simple criterion testing the validity of a Markov approximation appears very desirable.

3. Spectral properties and ergodicity

In this section we study the spectral properties of stochastic processes and their correlation functions, which characterize the dynamics of the system. Since the asymptotic behaviour for long times depends on the ergodic properties, we also discuss ergodicity problems.

3.1. Linearized theory of fluctuations

If the fluctuations about the deterministic motion of the system are small, their correlations may be calculated in linear response theory. This approximation corresponds closely to the "random-phase

approximation" which is extensively used in the theory of cooperative phenomena in various fields [71–74]. We give here a brief presentation of this method.

We describe the system by a Langevin equation (2.4.2)

$$\dot{x}(t) = v(x(t), t) + X(t) \tag{3.1.1}$$

with state-independent stochastic forces $X(t)$ (additive noise) satisfying (compare (2.4.17, 19))

$$\langle X(t) \rangle = 0 \tag{3.1.2a}$$

$$\langle X(t)\, X(s) \rangle = 2\mathbf{D}(t)\, \delta(t-s)\,. \tag{3.1.2b}$$

The stochastic forces give rise to fluctuations $\xi(t) = x(t) - a(t)$ about the deterministic motion $a(t)$. In linear response, one obtains

$$\xi(t) = \int_{-\infty}^{+\infty} \chi(t, s) \cdot X(s)\, \mathrm{d}s \tag{3.1.3}$$

where $\chi(t, s)$ is the susceptibility tensor of the deterministic system (containing a factor $\theta(t-s)$ to take care of the causality requirement). With (3.1.3), we obtain the two-time covariance matrix

$$\mathbf{S}(t_2, t_1) = \langle \xi(t_2)\, \xi^*(t_1) \rangle = 2 \int \chi(t_2, s) \cdot \mathbf{D}(s) \cdot \chi^{\dagger}(t_1, s)\, \mathrm{d}s\,. \tag{3.1.4}$$

For a stationary process with $\chi(t_2, t_1) = \chi(t_2 - t_1)$, $\mathbf{D}(t) = \mathbf{D} = \text{const.}$, one finds

$$\mathbf{S}(\tau) = 2 \int \chi(\tau + \tau') \cdot \mathbf{D} \cdot \chi^{\dagger}(\tau')\, \mathrm{d}\tau' \tag{3.1.5}$$

whose Fourier transform yields the spectral matrix

$$\mathbf{S}(\omega) = 2\chi(\omega) \cdot \mathbf{D} \cdot \chi^{\dagger}(\omega)\,. \tag{3.1.6}$$

Thus, in linear-fluctuation theory, the spectral properties of the correlations between fluctuations are expressed in terms of the spectral properties of the deterministic susceptibility. We assume a spectral representation

$$\chi(\tau) = \theta(\tau) \sum_n \chi_n \exp(-\mathrm{i}\omega_n \tau) \tag{3.1.7}$$

with Fourier transform

$$\chi(\omega) = \sum_n \frac{\chi_n}{\mathrm{i}(\omega_n - \omega)} \tag{3.1.8}$$

with eigenfrequencies having negative imaginary parts,

$$\operatorname{Im}\omega_n < 0\,, \tag{3.1.9}$$

to ensure stability of the deterministic state. With (3.1.7, 8) one obtains for the covariance matrix (3.1.5)

$$\mathbf{S}(\tau) = 2\sum_{n,n'} \frac{\boldsymbol{\chi}_n \cdot \mathbf{D} \cdot \boldsymbol{\chi}^{\dagger}_{n'}}{\mathrm{i}(\omega_n - \omega^*_{n'})} \exp(-\mathrm{i}\omega_n \tau) \qquad \tau > 0 \tag{3.1.10a}$$

$$= 2\sum_{n,n'} \frac{\boldsymbol{\chi}_n \cdot \mathbf{D} \cdot \boldsymbol{\chi}^{\dagger}_{n'}}{\mathrm{i}(\omega_n - \omega^*_{n'})} \exp(-\mathrm{i}\omega^*_n \tau) \qquad \tau < 0\,, \tag{3.1.10b}$$

and the spectral matrix (3.1.6) becomes

$$\mathbf{S}(\omega) = 2\sum_{n,n'} \frac{\boldsymbol{\chi}_n \cdot \mathbf{D} \cdot \boldsymbol{\chi}^{\dagger}_{n'}}{(\omega_n - \omega)(\omega^*_{n'} - \omega)}\,. \tag{3.1.11}$$

The linear-fluctuation approximation of this subsection breaks down when the fluctuations become large. This occurs in particular for "critical fluctuations" near phase transitions and instabilities where an eigenvalue of the deterministic susceptibility tensor $\boldsymbol{\chi}(\omega)$ diverges, either at $\omega = 0$ (soft-mode instability) or at $\omega \neq 0$ (hard-mode instability). A proper treatment of such cases requires non-perturbative methods to calculate spectral properties.

3.2. Spectral properties of time-homogeneous Markov process

We now proceed to a discussion of the spectral properties of a stochastic process independent of any assumption about the smallness of fluctuations.

The general characteristic of stochastic processes that information present in the distribution can never increase in the course of time, has important consequences for their time evolution. We restrict the following discussion to time-homogeneous Markov processes with propagators $R(t|s) = R(t-s)$. From the definition of the conditional probability there follow two "contraction" properties of $R^{\dagger}(\tau)$ and $R(\tau)$, respectively, which express the deterioration of information [75, 76]: The peaks and valleys of any state function $f(\boldsymbol{x})$ are never amplified by averaging, i.e. the amplitude of variation of the conditional average $\langle f(\boldsymbol{x}(t+\tau))|\boldsymbol{x}t\rangle$ never increases in the course of time,

$$\sup|\langle f(\boldsymbol{x}(t+\tau))|\boldsymbol{x}t\rangle| \equiv \sup\left|\int [R^{\dagger}(\tau) f](\boldsymbol{x})\,\mathrm{d}x\right| \tag{3.2.1}$$

$$\leq \sup|f(x)| \qquad \forall \tau > 0\,.$$

Further, given a stationary distribution p_{s} satisfying $R(\tau)\,p_{\mathrm{s}} = p_{\mathrm{s}}$, the "distance" of any $p(t)$ from p_{s} measured by the total variation of $|p(\boldsymbol{x}t) - p_{\mathrm{s}}(\boldsymbol{x})|$ never increases in the course of time,

$$\int |p(\boldsymbol{x}, t+\tau) - p_{\mathrm{s}}(\boldsymbol{x})|\,\mathrm{d}x \equiv \int |[R(\tau)\,(p(t) - p_{\mathrm{s}})](\boldsymbol{x})|\,\mathrm{d}x \tag{3.2.2}$$

$$\leq \int |p(\boldsymbol{x}t) - p_{\mathrm{s}}(\boldsymbol{x})|\,\mathrm{d}x \qquad \forall \tau > 0\,.$$

It is interesting to note that this property holds independently of whether $p(t)$ converges to p_s for $t \to \infty$.

Both the supremum in (3.2.1) and the total variation in (3.2.2) define norms in the appropriate Banach spaces, and the semigroups represented by $R^+(\tau)$ and $R(\tau)$ are therefore *contraction semigroups* [75, 76]. According to a theorem by Phillips and Lumer [75, 76], the master operator generates a contraction semigroup (with respect to the norm $\|f\| = \sqrt{\langle f^* f \rangle_s}$) if and only if it is *dissipative*, i.e.

$$\mathrm{Re}\langle f^* \Gamma^\dagger f \rangle_s = \mathrm{Re} \int f^*(\boldsymbol{x})\, (\Gamma^\dagger f)(\boldsymbol{x})\, p_s(\boldsymbol{x})\, \mathrm{d}x \leq 0 \tag{3.2.3}$$

for all f in the domain of $\Gamma^\dagger$. The average in (3.2.3) is taken over a stationary distribution p_s which is assumed to exist but not assumed to be unique (see section 3.4).

The eigenvalues λ of the master operator Γ coincide with those of $\Gamma^\dagger$, and are either real or occur in pairs λ, λ^*, because Γ is real. From (3.2.3) it follows that no eigenvalue lies in the right half of the complex plane,

$$\mathrm{Re}\,\lambda \leq 0 \qquad \forall \lambda\,. \tag{3.2.4}$$

The eigenfunctions ψ_λ of Γ and φ_λ of $\tilde{\Gamma} = \Gamma^\dagger$ form a bi-orthogonal set

$$\int \varphi_\lambda(\boldsymbol{x})\, \psi_{\lambda'}(\boldsymbol{x})\, \mathrm{d}x = 0 \quad \text{for } \lambda \neq \lambda'\,. \tag{3.2.5}$$

There exists at least one eigenvalue $\lambda_0 = 0$ with

$$\psi_0(\boldsymbol{x}) = p_s(\boldsymbol{x}), \qquad \varphi_0(\boldsymbol{x}) = 1 \quad \forall \boldsymbol{x} \text{ with } \Gamma(\boldsymbol{x}, \boldsymbol{y}) \neq 0 \tag{3.2.6}$$

whence

$$\int \psi_\lambda(\boldsymbol{x})\, \mathrm{d}x = 0, \qquad \int \varphi_\lambda(\boldsymbol{x})\, p_s(\boldsymbol{x})\, \mathrm{d}x = 0 \quad \forall \lambda \neq 0\,. \tag{3.2.7}$$

If $\lambda = 0$ is g-fold degenerate, there exists a bi-orthogonal basis $\{\psi_\gamma, \varphi_\gamma\}$ in the $\lambda = 0$ subspace such that all ψ_γ are probability distributions, $\psi_\gamma(\boldsymbol{x}) \geq 0$, $\int \psi_\gamma(\boldsymbol{x})\, \mathrm{d}x = 1$, and any stationary distribution can be written as a convex combination

$$p_s(\boldsymbol{x}) = \sum_\gamma p_\gamma\, \psi_\gamma(\boldsymbol{x}) \tag{3.2.8}$$

with weights $P_\gamma \geq 0$, $\Sigma_\gamma P_\gamma = 1$. This is connected with a topological structure of state space with respect to ergodic properties and asymptotic behaviour (see section 3.4). The right eigenfunctions ψ_n with $\lambda_n \neq 0$ have the significance of deviations from the stationary distribution which decay $\propto \exp(\lambda_n t)$. The left eigenfunctions φ_n belonging to $\lambda = 0$ are constants of motion; those belonging to $\lambda_n \neq 0$ represent stochastic variables whose statistical averages decay $\propto \exp(\lambda_n t)$.

We consider further the simple case that Γ and $\Gamma^\dagger$ have a discrete spectrum λ_n with a complete system of eigenfunctions ψ_n, φ_n with a normalization such that the orthonormality and completeness relations read

$$\int \varphi_m(x)\,\psi_n(x)\,\mathrm{d}x = \delta_{mn} \tag{3.2.9}$$

$$\sum_n \psi_n(x)\,\varphi_n(y) = \delta(x-y)\,. \tag{3.2.10}$$

Then there exist spectral representations of the kernel of Γ,

$$\Gamma(x,y) = \sum_n \lambda_n\,\psi_n(x)\,\varphi_n(y) \tag{3.2.11}$$

and of the conditional probability

$$R(x\tau|y0) = \sum_n \exp(\lambda_n\tau)\,\psi_n(x)\,\varphi_n(y)\,, \qquad \tau>0\,. \tag{3.2.12}$$

Thus, in the steady state characterized by p_s, the time correlation matrix of the set of random variables $f=(f_1, f_2, \ldots)$ can be written as

$$\mathbf{C}(\tau) = \langle f(t+\tau)\,f^*(t)\rangle_s = \sum_{n\geq 0} g_n h_n^* \exp(\lambda_n\tau), \qquad \tau>0\,, \tag{3.2.13}$$

with

$$g_n = \int f(x)\,\psi_n(x)\,\mathrm{d}x \tag{3.2.14}$$

$$h_n = \int f(x)\,\varphi_n(x)\,p_s(x)\,\mathrm{d}x \equiv \langle f\varphi_n\rangle_s\,. \tag{3.2.15}$$

The value for $\tau<0$ may be found from $\mathbf{C}(-\tau)=\mathbf{C}^\dagger(\tau)$ (see (1.2.18)). Since on account of (3.2.6) $g_0 = h_0 = \langle f\rangle_s$, the covariance matrix $\mathbf{S}(\tau)=\mathbf{C}(\tau)-\langle f\rangle_s\langle f^*\rangle_s$ is obtained from (3.2.13) by deleting the $n=0$ term,

$$\mathbf{S}(\tau) = \sum_{n\geq 1} g_n h_n^* \exp(\lambda_n\tau), \qquad \tau>0\,, \tag{3.2.16a}$$

$$= \sum_{n\geq 1} h_n^* g_n \exp(-\lambda_n\tau), \qquad \tau<0\,, \tag{3.2.16b}$$

and Fourier transformation yields the spectral matrix

$$\mathbf{S}(\omega) = \sum_{n\geq 1}\left[\frac{-g_n h_n^*}{\lambda_n + \mathrm{i}\omega} + \frac{-h_n g_n^*}{\lambda_n^* - \mathrm{i}\omega}\right]. \tag{3.2.17}$$

The long-time behaviour is determined by the eigenvalues with the smallest $|\mathrm{Re}\,\lambda|$. If the eigenvalue $\lambda=0$ is degenerate, the stationary distribution is non-unique (see (3.2.8)), and the system shows

zero-frequency anomalies [77–79]. In the case of a pair of purely imaginary eigenvalues $\lambda = \pm i\omega$ the system shows undamped oscillations of frequency ω (*finite-frequency anomalies*). If $\lambda_0 = 0$ is non-degenerate, and $\mathrm{Re}\,\lambda_n < 0 \quad \forall n > 0$, the long-time behaviour consists of a damped oscillation or an exponential decay, depending on whether $\mathrm{Im}\,\lambda_1 \neq 0$ or $=0$, respectively:

$$S(\tau) \propto \overset{\cos}{\sin}(\mathrm{Im}\,\lambda_1 \tau)\exp(\mathrm{Re}\,\lambda_1|\tau|)\,. \tag{3.2.18}$$

Of particular interest are the cases of metastability and of a stable limit cycle of the deterministic system. In the case of metastability, the stationary distribution has two peaks corresponding to the two stable deterministic states, and the long-time behaviour is characterized by a real eigenvalue λ_1 nearly degenerate with $\lambda_0 = 0$, with an eigenfunction describing a very slow relaxation of the metastable state towards the absolutely stable state [42, 80–87]. In section 6.3 such a case is discussed in detail. In the case of a limit cycle, the stationary distribution is peaked along the stable deterministic orbit, and the long-time behaviour is characterized by pairs of eigenvalues λ_n, λ_n^* with very small $|\mathrm{Re}\,\lambda_n|$ and with $\mathrm{Im}\,\lambda_n$ given by the frequency of the deterministic motion. The set of eigenfunctions describes slowly decaying perturbations travelling along the deterministic orbit.

A discrete spectrum with $\mathrm{Re}\,\lambda_n < 0 \quad \forall n > 0$ thus leads to an exponential long-time behaviour, at least as long as $\lambda = 0$ is not an accumulation point of eigenvalues $\lambda_n \neq 0$. Long-time tails with algebraic time dependence are obtained in the case of a continuous spectrum* extending without gap up to $\lambda = 0$. Assuming

$$\mathbf{S}(\tau) = \int_{-\infty}^{0} \mathbf{A}_{\pm}(\lambda)\exp(-|\lambda\tau|)\,\mathrm{d}\lambda\,, \qquad \tau \gtrless 0\,, \tag{3.2.19}$$

with an amplitude varying for $\lambda \to 0$ as

$$A(\lambda) \sim |\lambda|^{r-1}, \qquad r > 0\,, \tag{3.2.20}$$

yields an asymptotic behaviour with an algebraic long-time tail

$$S(\tau) \sim |\tau|^{-r}, \qquad |\tau| \to \infty\,. \tag{3.2.21}$$

In the case of a stochastic process in a discrete N-point state space, with a master operator represented by an $N \times N$ matrix Γ_{ij} with

$$\Gamma_{ij} \geq 0 (i \neq j), \qquad \Gamma_{ii} < 0, \qquad \sum_i \Gamma_{ij} = 0\,, \tag{3.2.22}$$

more detailed statements can be made about the spectrum [88, 89]:

– The spectrum of eigenvalues $\lambda(\Gamma)$ is contained in the union of n circular discs $|x - \Gamma_{ii}| \leq r_i$ with radii [88–90]

* In the presence of a continuous spectrum, the conditions of orthonormality (3.2.9) and completeness (3.2.10) have to be suitably generalized.

$$r_i = |\Gamma_{ii}|^{\alpha}\Big(\sum_{j\neq i}\Gamma_{ij}\Big)^{1-\alpha}, \qquad 0\leq\alpha\leq 1\,. \tag{3.2.23}$$

In particular, all eigenvalues are contained in the disc centered at $-\max|\Gamma_{ii}|$ with radius $\max|\Gamma_{ii}|$ (fig. 4). Thus, the real part of any nonzero eigenvalue is strictly negative, which rules out the possibility of recurring probability solutions with purely imaginary eigenvalues. If the union of discs (3.2.23) decomposes into disjoint subsets S_i consisting of N_i discs, each subset contains exactly N_i eigenvalues.

– If the eigenvalue $\lambda = 0$ is algebraically ν_0-fold degenerate, the rank of Γ is $N - \nu_0$, i.e. there exists a complete set of ν_0 linearly independent stationary distributions [91]. This is of importance in ergodic theory (see sections 3.3, 3.4).

– A birth and death process with strictly positive transition rates $w_{i,i+1}>0$, $w_{i+1,i}>0$, $w_{ij}=0$ $(j\neq i-1,\ i+1)$ has real nondegenerate eigenvalues [92]. Moreover, the $N-1$ eigenvalues $\bar{\lambda}$ of the truncated matrix $\bar{\Gamma}$ obtained by deleting the last row and column and putting $\bar{\Gamma}_{N-1,N-1} = -\Gamma_{N-2,N-1}$, separate those of Γ:

$$0=\lambda_0=\bar{\lambda}_0>\lambda_1>\bar{\lambda}_1\cdots>\bar{\lambda}_{N-2}>\lambda_{N-1}\,. \tag{3.2.24}$$

– If Γ is "doubly stochastic", $\Sigma_i\Gamma_{ij}=\Sigma_j\Gamma_{ij}=0$, there exists a uniform stationary distribution

$$p_s(i) = 1/N. \tag{3.2.25}$$

3.2.E1. Spectral properties of the two-state Markov process

For the generator (2.2.17) of the strictly stationary two-state process with $\dot{\rho}_0 = \text{const.} < 0$, $\dot{\alpha}_0 = \text{const.}$, one finds the eigenvalues

$$\lambda_0 = 0, \qquad \lambda_1 = \dot{\rho}_0 \tag{3.2.26}$$

with the eigenvectors

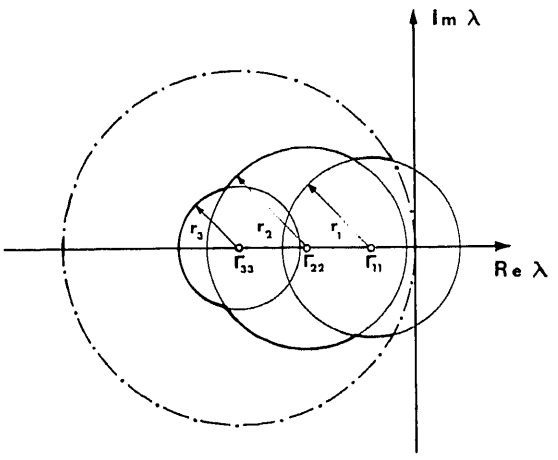

Fig. 4. Regions in the complex plane containing the eigenvalues of the master operator of a three-state Markov process ($|\Gamma_{11}|<|\Gamma_{22}|<|\Gamma_{33}|$). The dash-dotted circle is the border of the disc centered at $-|\Gamma_{33}|$ with radius $|\Gamma_{33}|$; the full circles are the borders of the discs centered at $-|\Gamma_{ii}|$ with radii given by (3.2.23) for $\alpha = 0$.

$$\psi_0(x) = \tfrac{1}{2}(1 + ax), \qquad \varphi_0(x) = 1$$
$$\psi_1(x) = \tfrac{1}{2}x, \qquad \varphi_1(x) = -a + x \tag{3.2.27}$$

where $a = -\dot{\alpha}_0/\dot{\rho}_0$ is the stationary value of $\langle x \rangle$ (see (2.2.27)). From the spectral representations (3.2.11) and (3.2.12) one recovers the generator (2.2.17) and the conditional probability (1.3.24) with $\rho(\tau)$ and $\alpha(\tau)$ given by (2.2.28, 29). The autocovariance and the spectral density of the fluctuations of the state variable x are found from (3.2.16, 17) in the form

$$s(\tau) = s \exp(-|\dot{\rho}_0|\tau) \tag{3.2.28}$$

$$s(\omega) = s \frac{2|\dot{\rho}_0|}{\dot{\rho}_0^2 + \omega^2} \tag{3.2.29}$$

where $s = 1 - a^2$ is the stationary value of the variance $\langle x^2 \rangle - \langle x \rangle^2$. The result (3.2.28) is in agreement with (1.3.28) and (2.2.28).

3.2.E2. Spectral properties of a Gauss–Markov process

The spectral analysis of the general stationary n-component Gauss–Markov is nontrivial. Here, we restrict the discussion to the case that the process factors into a product of one-component Gauss processes generated by

$$\Gamma = -\frac{\mathrm{d}}{\mathrm{d}x}(\dot{\rho}_0 x + \dot{\alpha}_0) + \tfrac{1}{2}\dot{\sigma}_0 \frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{3.2.30}$$

with values $\dot{\alpha}_0 = \text{const.}$, $\dot{\rho}_0 = \text{const.} < 0$, $\dot{\sigma}_0 = \text{const.} \geq 0$ which are generally different for different components. In section 4.4E1 it is shown that the case of a general Gauss–Markov process satisfying the conditions of strict detailed balance may be reduced to this case.

One has to distinguish principally between the cases $\dot{\rho}_0 < 0$ and $\dot{\rho}_0 = 0$. For $\dot{\rho}_0 < 0$, the spectrum is immediately obtained by noting the equivalence to the Schrödinger eigenvalue problem of a harmonic oscillator with

$$\hbar\omega = -\dot{\rho}_0, \qquad \hbar^2/m = \dot{\sigma}_0 \tag{3.2.31}$$

via the transformation (see eq. (4.3.21) below)

$$\Gamma^{\text{symm}} = \exp[(x-a)^2/4s]\, \Gamma \exp[-(x-a)^2/4s]$$
$$= \frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \tfrac{1}{2}m\omega^2(x-a)^2 + \tfrac{1}{2}\hbar\omega\,. \tag{3.2.32}$$

One finds the complete spectrum

$$\lambda_n = n\dot{\rho}_0, \qquad n = 0, 1, 2, \ldots \tag{3.2.33}$$

with

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \frac{1}{\sqrt{2\pi s}} H_n\left[\frac{x-a}{\sqrt{2s}}\right] \exp\left[-\frac{(x-a)^2}{2s}\right] \tag{3.2.34a}$$

$$\varphi_n(x) = \frac{1}{\sqrt{2^n n!}} H_n\left[\frac{x-a}{\sqrt{2s}}\right] \tag{3.2.34b}$$

where $H_n(x)$ are the Hermite polynomials, and $a = -\dot{\alpha}_0/\dot{\rho}_0$ and $s = -\dot{\sigma}_0/2\dot{\rho}_0$ are the stationary values of $\langle x\rangle$ and $\langle x^2\rangle - \langle x\rangle^2$, respectively (see (2.2.47, 48)).

The spectral representation (3.2.12) gives the expansion of the conditional probability (1.3.42) into exponentially damped modes. The autocovariance and the spectral density of the fluctuations of the state variable $x(t)$ are found from (3.2.16, 17) to be given by $\lambda_1 = \dot{\rho}_0$ alone,

$$s(\tau) = s \exp(-|\dot{\rho}_0 \tau|) \tag{3.2.35}$$

$$s(\omega) = s \frac{2|\dot{\rho}_0|}{\dot{\rho}_0^2 + \omega^2}. \tag{3.2.36}$$

The result (3.2.35) is in agreement with (1.3.47) and (2.2.46).

The eigenvalues λ_n are independent of the parameter $\dot{\sigma}_0$ and therefore of the variance s. In the limit $s \to 0$ corresponding to a pure drift $v = -\dot{\rho}_0 x$ the set of eigenfunctions degenerates into

$$\psi_n(x) = \delta^{(n)}(x), \qquad \varphi_n(x) = \frac{(-1)^n}{n!} x^n \tag{3.2.37}$$

which still formally satisfy the conditions of orthogonality (3.2.9) and completeness (3.2.10).

For $\dot{\rho}_0 = 0$ corresponding to a uniform Fokker–Planck-process, one obtains a continuous spectrum with non-normalizable eigenfunctions. If the spectrum is made discrete in the usual way by introducing periodic boundary conditions with period L one finds

$$\lambda_q = -i\dot{\alpha}_0 q - \tfrac{1}{2}\dot{\sigma}_0 q^2, \qquad q = \frac{2\pi}{L} l, \qquad l = 0, \pm 1, \ldots \tag{3.2.38}$$

$$\psi_q(x) = \frac{1}{L} \exp(iqx), \qquad \varphi_q(x) = \exp(-iqx), \tag{3.2.39}$$

but then the process is no longer Gaussian.

3.2.E3. Spectral properties of the process with independent increments

The stationary process with independent increments described by (2.3.25) also requires the specification of boundary conditions. For periodic boundary conditions with period L one finds

$$\lambda_q = \Gamma_q = \gamma[\rho(q) - 1], \qquad q = \frac{2\pi}{L} l, \qquad l = 0, \pm 1 \ldots \tag{3.2.40}$$

$$\psi_q(x) = \frac{1}{L} \exp(iqx), \qquad \varphi_q(x) = \exp(-iqx). \tag{3.2.41}$$

Here, $\rho(q) = \langle e^{-iqr} \rangle_\rho$ is the Fourier transform of the jump probability $\rho(r)$. In the drift-diffusion limit $\langle r^n \rangle_\rho = 0$ $(n > 2)$ one recovers the uniform Fokker–Planck process (3.2.38) with $\dot{\alpha}_0 = \gamma \langle r \rangle_\rho$, $\dot{\sigma}_0 = \gamma \langle r^2 \rangle_\rho$.

3.3. Ergodic properties

Ergodicity is concerned with the asymptotic behaviour of stochastic processes for $t \to \infty$, and with the closely related problem of determining the statistics of a stochastic process from a single realization. We restrict ourselves to the discussion of the ergodic nature of stochastic variables of a strictly stationary process $\boldsymbol{x}(t)$.

The set of stochastic variables $\{f_1(\boldsymbol{x}), f_2(\boldsymbol{x}), \ldots\}$ (not explicitly time-dependent) forming the vector variable $\boldsymbol{f}(\boldsymbol{x})$ is called ergodic if the time average

$$\bar{\boldsymbol{f}}^T = \frac{1}{2T} \int_{-T}^{T} \boldsymbol{f}(\boldsymbol{x}(t))\, \mathrm{d}t \tag{3.3.1}$$

tends to the ensemble average $\langle \boldsymbol{f} \rangle$ for $T \to \infty$. According to theorems by Birkhoff [93, 94] adapted to nondeterministic stochastic processes [76, 95], the limit

$$\bar{\boldsymbol{f}}^\infty = \lim_{T \to \infty} \frac{1}{2T} \int_{-T}^{T} \boldsymbol{f}(\boldsymbol{x}(t))\, \mathrm{d}t \tag{3.3.2}$$

considered as a random variable exists for almost all realizations $\boldsymbol{x}(t)$ and is independent of the reference time (chosen as $t = 0$ in (3.3.1)), provided $\boldsymbol{f}(\boldsymbol{x})$ is determined at all points $\boldsymbol{x} \in \Sigma$ and $\langle \boldsymbol{f} \rangle$ is finite. Thus, the stochastic vector variable $\boldsymbol{f}$ is ergodic if

$$\bar{\boldsymbol{f}}^\infty = \langle \boldsymbol{f} \rangle \text{ with probability 1} \tag{3.3.3a}$$

or equivalently if

$$\langle (\bar{\boldsymbol{f}}^\infty - \langle \boldsymbol{f} \rangle)(\bar{\boldsymbol{f}}^\infty - \langle \boldsymbol{f} \rangle)^* \rangle = 0\,. \tag{3.3.3b}$$

That this is a nontrivial requirement can be seen from the trivial example of a process with constant sample functions $x(t) = x$, where x is a random variable with nonvanishing variance. Then clearly $\bar{x}^\infty = x$ exists but does not equal $\langle x \rangle = a$ with probability 1. Of course it is always true that

$$\langle \bar{\boldsymbol{f}}^T \rangle = \langle \bar{\boldsymbol{f}}^\infty \rangle = \langle \boldsymbol{f} \rangle\,. \tag{3.3.4}$$

An equivalent criterion for ergodicity is obtained by expressing (3.3.3b) in terms of the covariance matrix $\mathbf{S}(\tau) = \langle \boldsymbol{f}(t+\tau) \boldsymbol{f}^*(t) \rangle - \langle \boldsymbol{f} \rangle \langle \boldsymbol{f}^* \rangle$,

$$\langle (\bar{\boldsymbol{f}}^T - \langle \boldsymbol{f} \rangle)(\bar{\boldsymbol{f}}^T - \langle \boldsymbol{f} \rangle)^* \rangle = \frac{1}{2T} \int_{-2T}^{2T} \left(1 - \frac{|\tau|}{2T}\right) \mathbf{S}(\tau)\, \mathrm{d}\tau\,. \tag{3.3.5}$$

It can be shown that

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-2T}^{2T}\left(1-\frac{|\tau|}{2T}\right)\mathbf{S}(\tau)\,\mathrm{d}\tau=\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\mathbf{S}(\tau)\,\mathrm{d}\tau \tag{3.3.6}$$

provided that the limit exists. Thus, the stochastic vector variable f is ergodic if and only if

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\mathbf{S}(\tau)\,\mathrm{d}\tau=\mathbf{0}\,. \tag{3.3.7}$$

From this criterion, one obtains two simple sufficient (but not necessary) conditions for ergodicity: The variable f is ergodic if its time correlation function satisfies

$$\langle f(t+\tau)\,f^*(t)\rangle\to\langle f\rangle\,\langle f^*\rangle\quad\text{for }\tau\to\infty\,, \tag{3.3.8}$$

or if its fluctuation has finite spectral density at zero frequency,

$$\mathbf{S}(\omega=0)<\infty\,. \tag{3.3.9}$$

The ergodicity condition (3.3.7) is certainly satisfied for a stochastic variable f of a stationary Markov process, if there exists a spectral representation (3.2.16) with eigenvalues $\lambda_n\neq 0$ $(n>0)$. If in addition $\mathrm{Re}\,\lambda_n<0$ $(n>0)$, even the stronger condition (3.3.8) holds.

Conditions for the ergodicity of the probability distribution can be cast into the same form by introducing the characteristic functions $f_{\mathrm{A}}(\boldsymbol{x})$ for measurable subsets $\mathrm{A}\subset\Sigma$,

$$\begin{aligned} f_{\mathrm{A}}(\boldsymbol{x})&=1 \quad \text{if } \boldsymbol{x}\in\mathrm{A}\\ &=0 \quad \text{if } \boldsymbol{x}\notin\mathrm{A}\,. \end{aligned} \tag{3.3.10}$$

The time average $\bar{f}^{\infty}_{\mathrm{A}}$ gives the fraction of time a given realization $\boldsymbol{x}(t)$ spends in A, the ensemble average $\langle f_{\mathrm{A}}\rangle$ gives the probability $p(\mathrm{A})=\int_{\mathrm{A}}p(\boldsymbol{x})\,\mathrm{d}x$, and the time correlation function between f_{A} and f_{B} is related to the two-event probability by

$$\begin{aligned} \langle f_{\mathrm{A}}(t+\tau)\,f_{\mathrm{B}}(t)\rangle&=p^{(2)}(\mathrm{A},\,t+\tau;\,\mathrm{B},\,t)\\ &=\int_{(\mathrm{A}\times\mathrm{B})}p^{(2)}(\boldsymbol{x}t+\tau;\,\boldsymbol{x}'t)\,\mathrm{d}x\,\mathrm{d}x'\,. \end{aligned} \tag{3.3.11}$$

The ergodicity criterion for the single-event probability,

$$\bar{f}^{\infty}_{\mathrm{A}}=p(\mathrm{A})\text{ with probability 1} \tag{3.3.12}$$

for all measurable subsets $\mathrm{A}\subset\Sigma$, is equivalent to the condition of *weak mixing* [94]

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T} p^{(2)}(\mathrm{A}, t+\tau; \mathrm{B}, t)\,\mathrm{d}\tau = p(\mathrm{A})\,p(\mathrm{B}) \qquad \forall \mathrm{A}, \mathrm{B}\subset\Sigma, \tag{3.3.13a}$$

which is equivalent to

$$\lim_{T\to\infty}\frac{1}{T}\int_{0}^{T} R(xt+\tau|yt)\,\mathrm{d}\tau = p(x) \qquad \forall x, y\in\Sigma \tag{3.3.13b}$$

for the type of system under consideration. A sufficient (but not necessary) condition for ergodicity of $p(x)$ is given by the *strong mixing* property of the two-event probability

$$\lim_{\tau\to\infty} p^{(2)}(\mathrm{A}, t+\tau; \mathrm{B}, t) = p(\mathrm{A})\,p(\mathrm{B}) \qquad \forall \mathrm{A}, \mathrm{B}\subset\Sigma \tag{3.3.14a}$$

or equivalently

$$\lim_{\tau\to\infty} R(x, t+\tau|yt) = p(x) \qquad \forall x, y\in\Sigma\,. \tag{3.3.14b}$$

In the case of a time-homogeneous Markov process with a propagator $R(\tau)$ having a spectral representation (3.2.12) with nondegenerate eigenvalue $\lambda_0 = 0$, the distribution $p = \psi_0$ is ergodic in the sense of (3.3.13). If in addition $\mathrm{Re}\,\lambda_n < 0$ $(n > 0)$, even the strong mixing condition (3.3.14) is satisfied.

Clearly, all stochastic variables $f(x)$ with $\langle f\rangle < \infty$ are ergodic if the single-event probability is ergodic.

The main ergodic theorem of Birkhoff relates ergodicity to the properties of time evolution in state space Σ. One introduces the concept of invariant irreducible subsets of Σ. A measurable subset $\mathrm{A}\subset\Sigma$ is called *invariant* if all sample functions with values $x(t_0)\in\mathrm{A}$ for a fixed time t_0 stay in A for all $t > t_0$ with probability 1. An invariant subset A is called *irreducible* if it contains no proper subsets which are both measurable and invariant. Then the Birkhoff theorem states:

> The probability distribution in the invariant subset A is ergodic if and only if A is irreducible. In particular, if Σ is irreducible, then the probability distribution is ergodic in Σ.

It is also of interest to study the ergodicity of products $\mathbf{F}_\tau(x(t+\tau),\ x(t)) = f(x(t+\tau))\,g(x(t))$ of random variables at different times. $\mathbf{F}_\tau$ is called ergodic if the time average

$$\bar{\mathbf{F}}_\tau^T = \frac{1}{2T}\int_{-T}^{T} f(x(t+\tau))\,g(x(t))\,\mathrm{d}t \tag{3.3.15}$$

tends for $T\to\infty$ to the correlation matrix

$$\mathbf{C}(\tau) = \langle f(t+\tau)\,g(t)\rangle\,. \tag{3.3.16}$$

A necessary and sufficient condition for the ergodicity of $\mathbf{F}_\tau$ is given by

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\langle f(t+\sigma+\tau)\,g(t+\sigma)\,f(t+\tau)\,g(t)\rangle\,\mathrm{d}\tau=\langle f(t+\tau)\,g(t)\rangle\langle f(t+\tau)\,g(t)\rangle\,. \tag{3.3.17}$$

This shows that the ergodicity of multiple-time products is related to the behaviour of higher-order correlation functions and thus to the ergodicity of multivariate probability distributions, and is in the case of non-Markov processes not automatically guaranteed by the ergodicity of the single-event distribution. An exception is the case of a strictly stationary Gauss process $x(t)$ for which the condition

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T}\langle x(\tau)\,x(0)\rangle\,\mathrm{d}\tau=\langle x\rangle\langle x\rangle \tag{3.3.18}$$

is necessary and sufficient for ergodicity of any random function $f(x(t_1),\ldots,x(t_n))$ [96, 97].

3.4. *Asymptotic behaviour*

In most applications one is interested in the stochastic behaviour of an aged system, where the time t of observation is much later than the time t_0 of preparation. It is often assumed without proof or justified by nonrigorous arguments only that the distribution $p(t)$ approaches some unique asymptotic distribution as $t\to\infty$.

In order to investigate the asymptotic behaviour of a general time-inhomogeneous process, it is more convenient to study the limit $t_0\to-\infty$ for a fixed time t of observation. We consider a system prepared at time t_0 with initial distribution p_0, and examine the behaviour of its distribution $p(t;t_0,p_0)$ at time t for $t_0\to-\infty$. If

$$p_{\mathrm{as}}(t)=\lim_{t_0\to-\infty}p(t;t_0,p_0) \tag{3.4.1}$$

exists and is independent of p_0, the process $x(t)$ is called *asymptotically stable*. This is the case if $\lim_{t_0\to-\infty}R(t|t_0)$ exists and represents a singular operator mapping the whole space $\Pi^*(\Sigma)$ on the unique element $p_{\mathrm{as}}(t)\in\Pi^*(\Sigma)$ given by

$$p_{\mathrm{as}}(xt)=\lim_{t_0\to-\infty}R(xt|yt_0)\,. \tag{3.4.2}$$

If p_{as} is time-independent, the process is *asymptotically stationary*.

We restrict the following considerations to time-homogeneous Markov processes with $R(t|t_0)=R(t-t_0)$. Then, any asymptotically stable process is automatically asymptotically stationary. Further, the asymptotic stability condition (3.4.2) is equivalent to the condition (3.3.14b) of strong mixing, and thus implies ergodicity of the distribution p_{as}. The reverse does not hold: For an ergodic distribution which is only weakly mixing [93, 94] the limit (3.4.2) does not exist independently of y.

In the following, we discuss the asymptotic behaviour assuming a spectral representation (3.2.12) for the propagator $R(\tau)$. The asymptotic properties are then determined by the eigenvalues with $\mathrm{Re}\,\lambda=0$. If there exist pairs of purely imaginary eigenvalues, the limit (3.4.2) does not exist, and the process is

asymptotically unstable. We exclude this case of undamped oscillations, assuming $\mathrm{Re}\,\lambda < 0$ for all $\lambda \neq 0$. If $\lambda_0 = 0$ is nondegenerate, the process is asymptotically stable, and p_{as} coincides with the right eigenfunction ψ_0 belonging to $\lambda_0 = 0$. If $\lambda = 0$ is g-fold degenerate, p_{as} exists and is of the form (3.2.8) with weights $P_\gamma = \int \varphi_\gamma(x)\, p_0(x)\, dx$ depending on p_0, i.e. the process is not asymptotically stable in the whole state space Σ.

The structure of the conditional probability $R(x\tau|y0)$ gives rise to a topological decomposition of state space Σ into *ergodicity classes* reflecting the asymptotic behaviour of the process. It can be seen from the spectral representation (3.2.12) that for any pair of states (x, y), the conditional probability $R(x\tau|y0)$ is either identically zero or strictly positive for all $\tau \in (0, \infty)$. Further, if for given (x, y) there exists a state such that both transitions $y \to z$ and $z \to x$ have positive probabilities, the same holds for the transition $y \to x$ on account of the Chapman–Kolmogorov–Smoluchowski equation (1.3.15).

Thus, the state space may be decomposed into a set of *irreducible ergodic classes* Σ_γ $(\gamma = 1, 2, \ldots)$, and a remaining class Σ' of *evanescent states*,

$$\Sigma = \bigcup_\gamma \Sigma_\gamma \cup \Sigma' . \tag{3.4.3}$$

An ergodic class Σ_γ is a set of states which are connected pair-wise in both directions by positive transition probabilities $R(x\tau|y0)$ but do not feed into any state outside Σ_γ:

$$\begin{aligned} &R(x\tau|y0) > 0 \qquad \forall x, y \in \Sigma_\gamma \\ &R(zt|y0) = 0 \qquad \forall y \in \Sigma_\gamma, \quad z \in \Sigma - \Sigma_\gamma . \end{aligned} \tag{3.4.4}$$

The class Σ' consists of the remaining states which are not fed from any state outside Σ' but feed into at least one state outside Σ':

$$\begin{aligned} &R(x\tau|z0) = 0 \qquad \forall x \in \Sigma', \quad z \in \Sigma - \Sigma' \\ &R(z\tau|y0) > 0 \qquad \forall y \in \Sigma' \quad \text{for some } z \in \Sigma - \Sigma' . \end{aligned} \tag{3.4.5}$$

Figure 5 shows a few examples of ergodicity classes. It should be noted that a continuous state space will in general contain lower-dimensional submanifolds as ergodicity classes. The boundary of an ergodic class, for instance, may form a separate ergodic class, or belong to the evanescent class.

From the Chapman–Kolmogorov–Smoluchowski equation (1.3.15) and the conservation of probability it can be seen that the probability for the transition $y \to x$ between states of the same ergodic class Σ_γ approaches a unique strictly positive asymptotic distribution $p_{as,\gamma}$ in Σ_γ, whereas the probability for any transition into an evanescent state approaches zero. Thus, the process is asymptotically stable and therefore ergodic within each of the ergodic classes Σ_γ. The asymptotic distributions $p_{as,\gamma}$ are just the right basis functions ψ_γ of the $\lambda = 0$ subspace used in (3.2.8),

$$\psi_\gamma(x) = p_{as,\gamma}(x) = \lim_{\tau \to \infty} R(x\tau|y0), \qquad y \in \Sigma_\gamma . \tag{3.4.6}$$

From the spectral representation (3.2.12) it follows that the corresponding left basis functions $\varphi_\gamma(y)$ describe the total asymptotic weight of transitions starting in y and feeding into Σ_γ,

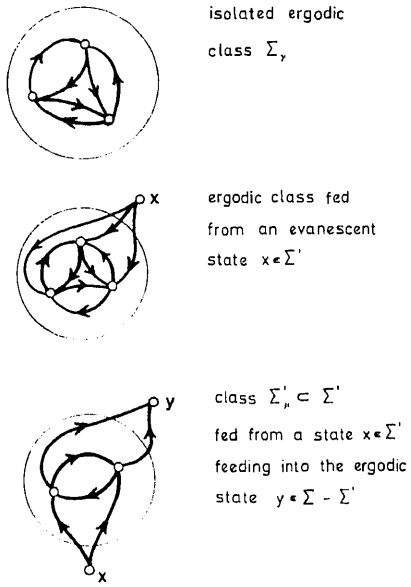

Fig. 5. Examples of various ergodicity classes.

$$\varphi_\gamma(y) = \lim_{t\to\infty} \int_{\Sigma_\gamma} R(x\tau|y0)\,\mathrm{d}x \tag{3.4.7}$$

whence

$$\sum_\gamma \varphi_\gamma(y) = 1 \qquad \forall y \in \Sigma. \tag{3.4.8}$$

Thus, the number of ergodic classes coincides with the degeneracy g of the eigenvalue $\lambda = 0$, the process within each of the ergodic classes Σ_γ has nondegenerate eigenvalue $\lambda = 0$, and the basis functions satisfy

$$\begin{aligned} \psi_\gamma(x) &> 0 \qquad \forall x \in \Sigma_\gamma \\ &= 0 \qquad \forall x \in \Sigma - \Sigma_\gamma \end{aligned} \tag{3.4.9a}$$

$$\begin{aligned} \varphi_\gamma(y) &= 1 \qquad \forall y \in \Sigma_\gamma \\ &= 0 \qquad \forall y \in \Sigma_{\gamma'}, \quad \gamma' \neq \gamma \\ &\geq 0 \qquad \forall y \in \Sigma'. \end{aligned} \tag{3.4.9b}$$

The eigenmodes belonging to any of the other eigenvalues $\lambda_n \neq 0$ may also be chosen in such a way that they describe a process which proceeds either within one of the Σ_γ or $\Sigma_\gamma \cup \Sigma'$, or in Σ' alone. The asymptotic probability for the transition from an evanescent state $y \in \Sigma'$ into the ergodic class Σ_γ is given by the left eigenfunction $\varphi_\gamma(y)$.

Any initial distribution p_0 can be written as a convex combination

$$p_0(x) = \sum_\gamma P_{0\gamma}\, p_{0\gamma}(x) + P'_0 p'_0(x) \tag{3.4.10}$$

$$P_{0\gamma},\, P'_0 \geq 0, \qquad \sum_\gamma P_{0\gamma} + P'_0 = 1$$

of distributions in the ergodicity classes Σ_γ, Σ', with weights $P_{0\gamma}$, P'_0. Each of the weights P_γ of the asymptotic distribution

$$p_{\mathrm{as}}(x) = \sum_\gamma P_\gamma\, \psi_\gamma(x) \tag{3.4.11}$$

consists of the initial weight $P_{0\gamma}$, plus a contribution from the initial weight P'_0 of the evanescent class:

$$P_\gamma = P_{0\gamma} + P'_0 \int_{\Sigma'} \varphi_\gamma(y)\, p'_0(y)\, \mathrm{d}y\,. \tag{3.4.12}$$

In the case of a discrete state space, the decomposition into ergodicity classes is reflected in the algebraic structure of the matrix Γ. The states may be renumbered such that Γ takes the form

$$\Gamma = \begin{bmatrix} \Gamma_1 & & 0 & B_1 \\ & \ddots & & \vdots \\ 0 & & \Gamma_g & B_g \\ 0 & & & B' \end{bmatrix}. \tag{3.4.13}$$

Here, each of the Γ_γ is an irreducible submatrix with nondegenerate eigenvalue $\lambda = 0$, describing the stochastic process within the ergodic class Σ_γ, the submatrix B' with $\det B' \neq 0$ describes the transitions between evanescent states, and the B_γ describe the transitions from evanescent states into the ergodic classes.

The decomposition of a discrete state space into ergodicity classes may be extended to the case that no complete bilinear set of eigenfunctions exists, by making use of the Jordan canonical form of the matrix Γ [26].

Asymptotic stability may also be tested with the help of a *Lyapunov-functional* $\mathscr{L}: \Pi^*(\Sigma) \to \mathbb{R}$: if there exists a strictly decreasing Lyapunov-functional,

$$\left.\begin{aligned} \mathscr{L}[p] &\geq 0 \\ \frac{\mathrm{d}}{\mathrm{d}t}\mathscr{L}[p] &\leq 0 \end{aligned}\right\} \quad \forall\, p \in \Pi^*(\Sigma) \tag{3.4.14}$$

$$= 0 \qquad \text{only for a unique } p = p_{\mathrm{as}}\,,$$

then the process is asymptotically stable. In the case of a stochastic process on a discrete state space with nondegenerate eigenvalue $\lambda_0 = 0$, Schlögl [98, 99] has introduced the *information gain*

$$K[p, p_s] = \sum_x p(xt) \ln[p(xt)/p_s(x)] \tag{3.4.15}$$

as a Lyapunov functional.

4. Symmetries and detailed balance

This section is devoted to an investigation of symmetry aspects of stochastic processes. The discussion of symmetry properties under transformations of state space follows similar lines as for deterministic systems. The formulation of the behaviour under time reversal, on the other hand, requires special care because of the conflicting aspects of macroscopic irreversibility and microscopic reversibility. Of particular importance and usefulness is the symmetry of "detailed balance" which has its origin in microscopic reversibility, and of generalizations thereof, and which is therefore discussed in detail.

4.1. Symmetry group of a stochastic process

In this subsection, we study the symmetry properties of a time-homogeneous Markov process under transformations of state space Σ. Let $\bar{x} = S(x)$ be a volume-conserving transformation of Σ. In the case of a discrete state space, S represents a permutation of its points. In the case of a continuous state space, any continuous S may be locally decomposed into a translation, a rotation, and a shear. Such a transformation $S: \Sigma \to \Sigma$ generates a transformation $O_S: \Pi(\Sigma) \to \Pi(\Sigma)$ of function space $\Pi(\Sigma)$ defined by

$$\bar{p}(\bar{x}t) = (O_S p)(\bar{x}t) = p(S^{-1}(\bar{x}), t) \equiv p(xt), \tag{4.1.1}$$

which because of $d\bar{x} = dx$ holds both for state functions and for probability densities.*

To the master operator Γ of the original process $x(t)$ there corresponds the master operator

$$\bar{\Gamma} = O_S \Gamma O_S^{-1} \tag{4.1.2}$$

of the transformed process $\bar{x}(t)$ with kernel

$$\bar{\Gamma}(\bar{x}, \bar{y}) = \Gamma(S^{-1}(\bar{x}), S^{-1}(\bar{y})) \equiv \Gamma(x, y). \tag{4.1.3}$$

S is called a *symmetry transformation* of the process if it leaves Γ invariant,

$$\bar{\Gamma} = \Gamma, \quad \text{i.e.} \quad \Gamma O_S = O_S \Gamma. \tag{4.1.4}$$

* In the case of non volume-conserving transformations S, the Jacobian has to be taken into account in (4.1.1).

The propagator $R(\tau)$ is then also invariant under S, i.e. the conditional probability satisfies

$$R(x\tau|y0) = R(S(x)\,\tau|S(y)\,0) \equiv R(\bar{x}\tau|\bar{y}0)\,. \tag{4.1.5}$$

The set of all symmetry transformations forms the *symmetry group* $\mathcal{G}$ of the process.

We now discuss the symmetry properties of the decomposition of phase space into ergodicity classes discussed in the previous section. The ergodic class Σ_γ is left invariant by a subgroup $\mathcal{H}_\gamma$ of $\mathcal{G}$,

$$\mathcal{H}_\gamma = \{S \in \mathcal{G} | S\Sigma_\gamma = \Sigma_\gamma\}\,. \tag{4.1.6}$$

The transformation of Σ_γ subduced by an element $S \in \mathcal{H}_\gamma$ is a symmetry transformation of the process in Σ_γ, i.e. the corresponding operator $O_S: \Pi(\Sigma_\gamma) \to (\Sigma_\gamma)$ commutes with the stochastic operator Γ_γ. Consequently, the symmetry group $\mathcal{G}_\gamma$ of the process in Σ_γ is at least the group $\mathcal{K}_\gamma$ subduced by $\mathcal{H}_\gamma$,

$$\mathcal{K}_\gamma = \mathcal{H}_\gamma / \mathcal{F}_\gamma\,, \tag{4.1.7}$$

where $\mathcal{F}_\gamma \subset \mathcal{H}_\gamma$ consists of those transformations $S \in \mathcal{H}_\gamma$ which leave every state of Σ_γ invariant. On the other hand, the symmetry group $\mathcal{G}_\gamma$ of Σ_γ may contain other symmetry operations not subduced by elements of $\mathcal{G}$.

The subgroup $\mathcal{H}_\gamma$ generates the *left-coset decomposition*

$$\mathcal{G} = \mathcal{H}_\gamma \oplus S_2\mathcal{H}_\gamma \oplus \cdots \oplus S_n\mathcal{H}_\gamma \tag{4.1.8}$$

where n is the index of $\mathcal{H}_\gamma$ in $\mathcal{G}$. A coset element $S \in S_\nu\mathcal{H}_\gamma$ transforms the ergodic class Σ_γ into a symmetry-related replica $\Sigma_{\gamma'}$ with symmetry group

$$\mathcal{G}_{\gamma'} = S_\nu \mathcal{G}_\gamma S_\nu^{-1} \tag{4.1.9}$$

isomorphous to $\mathcal{G}_\gamma$. As a consequence, either $\mathcal{H}_\gamma$ coincides with $\mathcal{G}$, in which case the ergodic class Σ_γ is fully invariant under $\mathcal{G}$, or Σ_γ is a member of a *star* Σ_{γ^*} of n symmetry-related ergodic classes with conjugate symmetry groups (4.1.9). Conversely, an ergodic class Σ_γ which is inequivalent to any other class must be fully invariant under $\mathcal{G}$. Clearly, the evanescent class Σ' is fully invariant under $\mathcal{G}$.

The asymptotic distributions $p_{\mathrm{as},\gamma} = \psi_\gamma$ transform according to irreducible representations of $\mathcal{G}$. Each ψ_γ is invariant under the symmetry group $\mathcal{G}_\gamma$,

$$\psi_\gamma(\bar{x}) \equiv \psi_\gamma(S(x)) = \psi_\gamma(x) \qquad \forall S \in \mathcal{G}_\gamma\,. \tag{4.1.10}$$

The same holds on account of (1.3.14) for all multivariate distributions $p^{(k)}_{\mathrm{as},\gamma}$ in Σ_γ. Consequently,

$$\langle f_1(x_1 t_1) \cdots f(x_k t_k)\rangle = \langle f_1(\bar{x}_1 t_1) \cdots f_n(\bar{x}_k t_k)\rangle \quad \forall x_1, \ldots, x_k \in \Sigma_\gamma, \quad S \in \mathcal{G}_\gamma \tag{4.1.11a}$$

i.e.

The nonzero part of any correlation function in Σ_γ is fully symmetric under $\mathcal{G}_\gamma$. (4.1.11b)

An asymptotic distribution $p_{\rm as} = \Sigma_\gamma P_\gamma \psi_\gamma$ with arbitrary weights P_γ has in general no symmetry properties, but for each star Σ_{γ^*} of symmetry-related classes Σ_γ one may form the fully symmetric convex combination with equal weights $P_\gamma = 1/n$,

$$p_{\rm symm} = \frac{1}{n} \sum_{\gamma \in \gamma^*} \psi_\gamma \tag{4.1.12}$$

which is invariant under the symmetry group of the star,

$$\mathcal{G}_{\gamma^*} = \bigoplus_{\gamma \in \gamma^*} \mathcal{G}_\gamma . \tag{4.1.13}$$

4.2. Time-reversal properties of a stochastic process

For any process σ (Markovian or non-Markovian) with sample functions $\boldsymbol{x}(t)$, $t \in [t_0, \infty)$, and for any set of time instants $S \cup T = \{s_1, \ldots, s_m, t_1, \ldots, t_n\}$ with $t_0 \le s_1 < \cdots < s_m < t_1 < \cdots < t_n < \infty$ and a corresponding set of state vectors $\boldsymbol{Y} \cup \boldsymbol{X}$, one may define *retarded* and *advanced* conditional probabilities $\overrightarrow{R}_\sigma^{(n|m)}(T|S)$ and $\overleftarrow{R}_\sigma^{(n|m)}(T|S)$ by

$$p_\sigma^{(n+m)}(\boldsymbol{XT}, \boldsymbol{YS}) = \overrightarrow{R}_\sigma^{(n|m)}(\boldsymbol{XT}|\boldsymbol{YS})\, p_\sigma^{(m)}(\boldsymbol{YS}) \tag{4.2.1}$$

$$= \overleftarrow{R}_\sigma^{(m|n)}(\boldsymbol{YS}|\boldsymbol{XT})\, p_\sigma^{(n)}(\boldsymbol{XT}) . \tag{4.2.2}$$

In the previous sections, only the retarded probabilities $\overrightarrow{R}$ have been used.

With any process σ one may associate a time-reversed process $\hat{\sigma}$ containing the time-reversed sample functions $\widehat{x(t)} = \hat{x}(-t) \in \hat{\sigma}$, $t \in (-\infty, \hat{t}_0 = -t_0]$, with the same measure in function space as was associated with $x(t) \in \sigma$. Here $\hat{x}$ is the coordinate obtained by time reversal from the coordinate x. The retarded and advanced conditional probabilities of $\hat{\sigma}$ defined for $-\infty < s_1 < \cdots < s_m < t_1 < \cdots < t_n \le \hat{t}_0$ by

$$p_{\hat{\sigma}}^{(n+m)}(\hat{\boldsymbol{X}}\hat{T}, \hat{\boldsymbol{Y}}S) = \overrightarrow{R}_{\hat{\sigma}}^{(n|m)}(\hat{\boldsymbol{X}}\hat{T}|\hat{\boldsymbol{Y}}S)\, p_{\hat{\sigma}}^{(m)}(\hat{\boldsymbol{Y}}S) \tag{4.2.3}$$

$$= \overleftarrow{R}_{\hat{\sigma}}^{(m|n)}(\hat{\boldsymbol{Y}}S|\hat{\boldsymbol{X}}\hat{T})\, p_{\hat{\sigma}}^{(n)}(\hat{\boldsymbol{X}}\hat{T}) \tag{4.2.4}$$

are related to those of σ by

$$\overrightarrow{R}_{\hat{\sigma}}(\hat{\boldsymbol{X}}\hat{T}|\hat{\boldsymbol{Y}}S) = \overleftarrow{R}_\sigma(\hat{\boldsymbol{X}} - T|\hat{\boldsymbol{Y}} - S) \tag{4.2.5}$$

where $-T = \{-t_1, \ldots, -t_n\}$, $-S = \{-s_1, \ldots, -s_m\}$.

Processes ω and α satisfying

$$\overrightarrow{R}_\omega^{(n|m)}(T|S) = \overrightarrow{R}_\omega^{(n|1)}(T|s_{\max}) \tag{4.2.6}$$

and

$$\overleftarrow{R}_{\alpha}^{(n|m)}(S|T) = \overleftarrow{R}_{\alpha}^{(n|1)}(S|t_{\min}) \tag{4.2.7}$$

for all S, T with $s_{\max} < t_{\min}$ are called *retarded-Markovian* (or simply Markovian) and *advanced-Markovian*, respectively. With these definitions, we have the following theorem:

If σ is retarded-Markovian, then $\hat{\sigma}$ is advanced-Markovian,
and vice-versa. (4.2.8)

In this context it is important to note that the linear continuation of $\overrightarrow{R}_{\sigma}^{(1|1)}(t|s) = \overrightarrow{R}_{\sigma}(t|s)$, $t > s$ defines a linear operator describing the forward propagation of a whole class $C^{>}$ of forward-Markovian processes generated by different initial distributions $p(t_0)$. It is this whole class $C^{>}$ which constitutes a Markov "process" as considered in this review. Similarly, the linear continuation of $\overleftarrow{R}_{\sigma}(t|s)$, $t < s$ describes the backward propagation of a class $C^{<}$ of backward-Markovian processes, generated by different final distributions $p(\hat{t}_0)$. In general, the classes $C^{>}$ and $C^{<}$ do not coincide. The class $C^{<}$ generated by final distributions has limited physical application, and its *anticausal* nature may easily lead to confusion.

In order to define time-reversal invariance, both processes σ and $\hat{\sigma}$ have to be defined on the same domain, i.e. on an interval $t_0 \leq t \leq \hat{t}_0 = -t_0 (t_0 < 0)$, or on the whole t-axis. Then, a process is called *time-reversal invariant* if $\sigma = \hat{\sigma}$, i.e. if the measure in function space is invariant under time reversal, or if the process σ contains the sample functions $\boldsymbol{x}(t)$ and $\hat{\boldsymbol{x}}(-t)$ with equal probability, or equivalently if

$$p^{(n)}(\boldsymbol{X}T) = p^{(n)}(\hat{\boldsymbol{X}} - T) \qquad \forall n . \tag{4.2.9}$$

A time-reversal invariant process σ which is forward Markovian is also backward Markovian and vice versa. However, it is important to note that the other members of the classes $C^{>}$ and $C^{<}$ generated by $\overleftrightarrow{R}_{\sigma}(t|s)$ of a time-reversal invariant Markovian process σ are in general not time-reversal invariant, and the intersection $C^{>} \cap C^{<}$ constitutes a very special class of processes. For instance, in the case of a time-homogeneous $\overleftrightarrow{R}_{\sigma}(\tau)$, only strictly stationary processes can be time-reversal invariant.

4.3. *Detailed-balance symmetry*

The time-reversal invariance of microscopic motion has important consequences for the macroscopic behaviour, as is clearly demonstrated by the principle of detailed balance for systems in thermodynamic equilibrium [3, 100] and by the Onsager reciprocity relations of irreversible thermodynamics [100–102].

In this subsection, we briefly review the origin of the principle of detailed balance and discuss possible generalizations for driven systems.

The microscopic Liouville motion $\boldsymbol{q}_t = \boldsymbol{q}(t)$ of the system in phase space $\Gamma = \{\boldsymbol{q}\}$ is described by the time-homogeneous propagator (see ref. [34])

$$R(\boldsymbol{q}\tau|\boldsymbol{q}_0 0) = \delta(\boldsymbol{q} - \boldsymbol{q}_\tau) . \tag{4.3.1}$$

From microscopic reversibility and time-homogeneity we find for the time-reversed motion

$$R(q\tau|q_0 0) = R(\hat{q}_0 0|\hat{q}\tau) = R(\hat{q}_0\tau|\hat{q}0) \qquad \forall q_0, q \in \Gamma, \tag{4.3.2}$$

where $\hat{q}$ is the coordinate related to q by time reversal (see fig. 6).

We consider a stationary distribution $\rho(q_\tau) = \rho(q_0)$. If q and $\hat{q}$ are on the same trajectory, i.e. if $\hat{q}_\tau = q_{\tau+\delta}$ for some δ, then

$$\rho(q) = \rho(\hat{q}) \qquad \forall q \in \Gamma. \tag{4.3.3}$$

If q_τ and $\hat{q}_\tau$ are not on the same trajectory, i.e. if there exists a constant of motion which is odd under time reversal (e.g. angular momentum), then we associate with the process σ under consideration the time-reversed process $\hat{\sigma}$. The same procedure is necessary if the motion occurs in an external field which is odd under time reversal. We then have instead of (4.3.2) and (4.3.3)

$$R_\sigma(q\tau|q_0 0) = R_{\hat{\sigma}}(\hat{q}_0\tau|\hat{q}0) \qquad \forall q_0, q \in \Gamma \tag{4.3.4}$$

$$\rho_\sigma(q) = \rho_{\hat{\sigma}}(\hat{q}) \qquad \forall q \in \Gamma \tag{4.3.5}$$

yielding the condition of detailed balance

$$p^{(2)}_\sigma(q\tau, q_0 0) = p^{(2)}_{\hat{\sigma}}(\hat{q} - \tau, \hat{q}_0 0) = p^{(2)}_{\hat{\sigma}}(\hat{q}_0\tau, \hat{q}0) \tag{4.3.6}$$

for the microscopic joint probability distribution, valid for any system in thermodynamic equilibrium.

The significance of this detailed-balance condition lies in the fact that it survives coarse-graining: The joint probability distribution $p^{(2)}(x\tau, y0)$ of the macrovariables $x = x(q)$ is given by the coarse-graining operation (1.2.6),

$$p^{(2)}(x\tau, y0) = \int \delta(x(q) - x)\, \delta(y(q') - y) \rho^{(2)}(q\tau, q'0)\, dq\, dq' . \tag{4.3.7}$$

One finds from (4.3.6) the detailed-balance condition

$$p^{(2)}_\sigma(x\tau, y0) = p^{(2)}_{\hat{\sigma}}(\hat{x} - \tau, \hat{y}0) = p^{(2)}_{\hat{\sigma}}(\hat{y}\tau, \hat{x}0) \qquad \forall x, y \in \Sigma \tag{4.3.8}$$

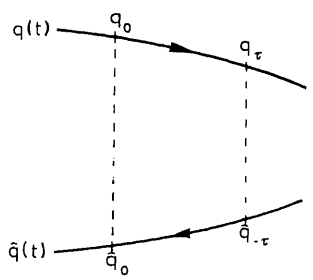

Fig. 6. Trajectory $q(t)$ and time-reversed trajectory $\hat{q}(t)$.

for the macrodistribution, again valid for any system in thermodynamic equilibrium. Integration over y yields the analog of (4.3.5),

$$p_\sigma(x) = p_{\hat{\sigma}}(\hat{x}) \qquad \forall x \in \Sigma . \tag{4.3.9}$$

Eq. (4.3.4), on the other hand, has no direct analog after coarse-graining. One only finds relation (4.2.5), i.e.

$$\vec{R}_\sigma(x\tau|y0) = \overleftarrow{R}_{\hat{\sigma}}(\hat{x}0|\hat{y}\tau) \tag{4.3.10}$$

between the retarded and advanced conditional probabilities.

Driven systems do not in general satisfy the detailed-balance condition (4.3.6): One is interested here in a situation where a system, which is driven by simultaneous coupling to several reservoirs, reaches a stationary state. As long as the reservoirs are considered finite, such a state can at best be quasi-stationary, but for sufficiently large reservoirs, the state will not change appreciably over a long period of time. Then, although the microdynamics in the phase space Γ_{tot} of the total system (system + reservoirs) is still microreversible in the sense of (4.3.4), the quasistationary distribution clearly violates the time-reversal symmetry (4.3.5), and therefore detailed balance (4.3.6) does not hold in Γ_{tot}. – Alternatively, one may eliminate the bath variables and obtain in the limit of infinite reservoirs a stationary distribution in the phase space Γ of the system. However, the process $\hat{\sigma}$ obtained by time-reversal from the process σ in phase space Γ is in general not identical with the process obtained by elimination of the reservoir variables from the time-reversed process in Γ_{tot}: In $\hat{\sigma}$, only the motion of the system variables (and not that of the bath variables!) is reversed. We thus conclude that detailed balance (4.3.6) is in general violated for the process in phase space Γ.

Under special conditions, one may of course have detailed balance on a coarse-grained level even though it is violated microscopically. Examples for such a situation are provided by models for the single-mode laser, hydrodynamic systems and chemical systems [3, 5, 8, 11, 12, 15, 18]. In this context it should be observed that the validity of (4.3.9) is necessary but not sufficient for detailed balance.

Since for driven systems, there is thus no microscopic basis for expecting a detailed-balance condition (4.3.8) relating the joint probability of a process σ to that of the time-reversed process $\hat{\sigma}$, it is meaningful to generalise the concept of detailed balance. We consider a pair of stationary processes $(\sigma, \bar{\sigma})$ satisfying a *generalized detailed-balance relation* of the form

$$\begin{aligned} p^{(2)}_\sigma = (x\tau, y0) &= p^{(2)}_{\bar{\sigma}}(\bar{x} - \tau, \bar{y}0) \\ &= p^{(2)}_{\bar{\sigma}}(\bar{y}\tau, \bar{x}0) \qquad \forall x, y \in \Sigma \end{aligned} \tag{4.3.11}$$

or

$$R_\sigma(x\tau|y0)\, p_\sigma(y) = R_{\bar{\sigma}}(\bar{y}\tau|\bar{x}0)\, p_{\bar{\sigma}}(\bar{x}) . \tag{4.3.12}$$

The process $\bar{\sigma}$ may be related to σ for instance by time reversal of the sample functions combined with a suitable transformation of the external fields, and we have allowed for a volume-conserving transformation

$$\bar{x} = \Theta \cdot x \tag{4.3.13}$$

of state space, consisting for instance of time reversal of the state variables combined with some rotation or reflection. (The explicit representation of such a transformation Θ is optional; it may always be absorbed into the definition of process $\bar{\sigma}$.)

Integration of (4.3.11) over y yields

$$p_\sigma(x) = p_{\bar{\sigma}}(\bar{x}) . \tag{4.3.14}$$

If (4.3.11) is satisfied for some transformation Θ, it is also satisfied for Θ^{-1}.

We do not investigate further the microscopic conditions for the existence of a generalised detailed-balance relation (4.3.11), but study some of its consequences. For a stationary Markov process, one obtains from (4.3.12) by using (1.3.14) for the n-point probability the relation

$$p_\sigma^{(n)}(XT) = p_{\bar{\sigma}}^{(n)}(\bar{X} - T) , \tag{4.3.15}$$

which implies corresponding symmetry relations for correlations tensors. In particular, one finds

$$S_{fg}(\tau) = \bar{S}_{\bar{g}\bar{f}}(\tau) = \bar{S}_{\bar{f}\bar{g}}(-\tau) , \tag{4.3.16}$$

where the state functions $\bar{f}$, $\bar{g}$ are defined by

$$\bar{f}(\bar{x}) = f(x), \bar{g}(\bar{x}) = g(x) .$$

For the kernels of the stochastic operators Γ_σ, $\Gamma_{\bar{\sigma}}$, one finds by differentiating (4.3.12) with respect to τ and observing (4.3.14) the condition of generalized detailed balance

$$\begin{aligned} \Gamma_\sigma(x, y)\, p_\sigma(y) &= \Gamma_{\bar{\sigma}}(\bar{y}, \bar{x})\, p_{\bar{\sigma}}(\bar{x}) \\ &= \Gamma_{\bar{\sigma}}(\bar{y}, \bar{x})\, p_\sigma(x) . \end{aligned} \tag{4.3.17}$$

By applying the transformation ($x \to \bar{x}$, $\sigma \to \bar{\sigma}$), observing (4.3.14), and interchanging x and y, one finds

$$\Gamma_\sigma(x, y) = \Gamma_{\bar{\sigma}}(\bar{\bar{x}}, \bar{\bar{y}}) \tag{4.3.18}$$

on the support p_σ, i.e. the process $\bar{\bar{\sigma}}$ differs from σ at most by a transformation of state space. Therefore, one may assume $\sigma = \bar{\bar{\sigma}}$, $\Theta^2 = \mathbf{1}$ without loss of generality.

It is interesting to note that (4.3.17) implies the stationarity of p_σ: If the equation is satisfied for some function ψ, i.e. if $\Gamma_\sigma(x, y)\, \psi(y) = \Gamma_{\bar{\sigma}}(y, x)\, \psi(x)$, then integration over y yields $\Gamma_\sigma \psi = 0$, which shows that ψ is a stationary solution of the master equation.

Eq. (4.3.17) gives rise to an interesting relation between the spectral properties of processes σ and $\bar{\sigma}$ [89]: Multiplication (4.3.17) by a left eigenfunction $\varphi_{\sigma n}(x)$ of Γ_σ to eigenvalue λ_n and integration over x shows that

$$\varphi_{\sigma n}(x)\, p_\sigma(x) \equiv \langle \bar{\varphi}_{\bar{\sigma} n} \varphi_{\sigma n} \rangle\, \psi_{\bar{\sigma} n}(\bar{x}) \tag{4.3.19a}$$

defines a properly normalized right eigenfunction $\psi_{\bar{\sigma} n}$ of $\Gamma_{\bar{\sigma}}$ to the same eigenvalue λ_n. Here, the

function $\bar{\varphi}_{n\bar{\sigma}}$ is defined by $\bar{\varphi}_{\bar{\sigma}n}(\boldsymbol{x}) = \varphi_{\bar{\sigma}n}(\bar{\boldsymbol{x}})$. Similarly, if $\varphi_{\bar{\sigma}n}(\bar{\boldsymbol{x}})$ is a left eigenfunction of $\Gamma_{\bar{\sigma}}$, then

$$\varphi_{\bar{\sigma}n}(\bar{\boldsymbol{x}})\, p_{\bar{\sigma}}(\bar{\boldsymbol{x}}) \equiv \langle \varphi_{\sigma n} \bar{\varphi}_{\bar{\sigma}n} \rangle\, \psi_{\sigma n}(\boldsymbol{x}) \tag{4.3.19b}$$

defines a right eigenfunction $\psi_{\sigma n}$ of Γ_{σ} to the same eigenvalue. The stationary distribution $p_{\sigma}(\boldsymbol{x}) = p_{\bar{\sigma}}(\bar{\boldsymbol{x}})$ is simultaneous right eigenfunction of Γ_{σ} and $\Gamma_{\bar{\sigma}}$ to $\lambda = 0$.

Of particular importance is the case of *strict detailed balance*: If $\Gamma_{\bar{\sigma}}(\bar{\boldsymbol{x}}, \bar{\boldsymbol{y}}) = \Gamma_{\sigma}(\boldsymbol{x}, \boldsymbol{y}) \quad \forall \boldsymbol{x}, \boldsymbol{y}$, i.e. if the process σ differs from $\bar{\sigma}$ at most by a transformation $\boldsymbol{\Theta}$ of state space, the condition (4.3.17) takes the simple form

$$\Gamma_{\sigma}(\boldsymbol{x}, \boldsymbol{y})\, p_{\sigma}(\boldsymbol{y}) = \Gamma_{\sigma}(\boldsymbol{y}, \boldsymbol{x})\, p_{\sigma}(\boldsymbol{x}) \,. \tag{4.3.20}$$

This case may always be reduced to the case $\sigma = \bar{\sigma}$, $\boldsymbol{\Theta} = \mathbf{1}$ by a redefinition of the process $\bar{\sigma}$. The condition (4.3.20) has the important consequence that the master operator Γ_{σ} becomes a symmetric operator under the scalar product $(f, g) = \int f(\boldsymbol{x})\, g(\boldsymbol{x})\, [p_{\mathrm{s}}(\boldsymbol{x})]^{-1}\, \mathrm{d}\boldsymbol{x}$, and has therefore only real eigenvalues λ. It may be explicitly symmetrised by the transformation

$$\Gamma^{\mathrm{symm}}(\boldsymbol{x}, \boldsymbol{y}) = [p_{\mathrm{s}}(\boldsymbol{x})]^{-1/2} \Gamma(\boldsymbol{x}, \boldsymbol{y})\, [p_{\mathrm{s}}(\boldsymbol{y})]^{+1/2} \,. \tag{4.3.21}$$

4.3.E1. Detailed balance of the two-state Markov process

The time-homogeneous two-state Markov process with generator (2.2.17),

$$\Gamma(x, y) = \tfrac{1}{2}(\dot{\alpha}_0 + \dot{\rho}_0 y) x \tag{4.3.22}$$

satisfies the condition (4.3.20) of strict detailed balance, as is verified immediately by noting that the stationary distribution is because of (2.2.27) given by

$$p_{\mathrm{s}}(x) = \frac{1}{2}\left(1 - \frac{\dot{\alpha}_0}{\dot{\rho}} x\right). \tag{4.3.23}$$

The master operator (4.3.22) may therefore be symmetrised by the transformation (4.3.21) yielding

$$\Gamma^{\mathrm{symm}}(x, y) = \tfrac{1}{4}\{\dot{\alpha}_0(\boldsymbol{x} + \boldsymbol{y}) + \dot{\rho}_0(1 + xy) + \sqrt{\dot{\rho}_0^2 - \dot{\alpha}_0^2}\,(1 - xy)\} \,. \tag{4.3.24}$$

Here, $\sqrt{\dot{\rho}_0^2 - \dot{\alpha}_0^2}$ is real on account of eq. (2.2.20).

4.4. Detailed balance of the Fokker–Planck process

Of particular interest are the consequences of generalized detailed balance for a stationary, asymptotically stable Fokker–Planck process defined by the differential operator (see (2.3.9))

$$\Gamma_{\sigma} = -\frac{\partial}{\partial \boldsymbol{x}} \cdot \boldsymbol{v}_{\sigma}(\boldsymbol{x}) + \frac{\partial^2}{\partial \boldsymbol{x}\, \partial \boldsymbol{x}} : \mathbf{D}_{\sigma}(\boldsymbol{x}) \tag{4.4.1a}$$

corresponding to the kernel (compare (2.4.18))

$$\Gamma_\sigma(x, y) = v_\sigma(y) \cdot \frac{\partial}{\partial y}\,\delta(y-x) + \mathbf{D}_\sigma(y) : \frac{\partial^2}{\partial y\,\partial y}\,\delta(y-x)\,. \tag{4.4.1b}$$

We restrict the consideration to transformations Θ satisfying

$$\Theta^2 = \mathbf{1}\,. \tag{4.4.2}$$

Under such a transformation (which is now explicitly assumed to be linear) the state space becomes the direct sum of an even and an odd invariant subspace, $\Sigma = \Sigma_g \oplus \Sigma_u$, such that

$$\bar{x} = \Theta \cdot x = \begin{cases} x & (x \in \Sigma_g) \\ -x & (x \in \Sigma_u)\,. \end{cases} \tag{4.4.3}$$

In a symmetry-adapted coordinate system, $\Theta_{ij} = \Theta_i \delta_{ij}$ with $\Theta_i = \pm 1$.

By observing the rule

$$f(y)\frac{\partial}{\partial x}\,\delta(y-x) = f(x)\frac{\partial}{\partial x}\,\delta(y-x) + \left(\frac{\partial}{\partial x} f(x)\right)\delta(y-x) \tag{4.4.4}$$

and noting that $\delta(\bar{y}-\bar{x}) = \delta(y-x)$, it follows that the detailed-balance relation (4.3.17) is equivalent to the set of three equations

$$(\mathbf{D}_\sigma - \Theta \cdot \mathbf{D}_{\bar{\sigma}} \cdot \Theta) p_\sigma = 0 \tag{4.4.5}$$

$$\tfrac{1}{2}(v_\sigma + \Theta \cdot v_{\bar{\sigma}}) p_\sigma - \frac{\partial}{\partial x} \cdot (\mathbf{D}_\sigma p_\sigma) = 0 \tag{4.4.6}$$

$$\frac{\partial}{\partial x} \cdot \left[v_\sigma p_\sigma - \frac{\partial}{\partial x} \cdot (\mathbf{D}_\sigma p_\sigma) \right] = 0\,. \tag{4.4.7}$$

It is convenient to introduce the stationary probability current

$$j_\sigma = v_\sigma p_\sigma - \frac{\partial}{\partial x} \cdot (\mathbf{D}_\sigma p_\sigma) \tag{4.4.8}$$

and its even and odd components

$$j_\sigma^+ = \tfrac{1}{2}(j_\sigma + \Theta \cdot j_{\bar{\sigma}}) \tag{4.4.9}$$

$$j_\sigma^- = \tfrac{1}{2}(j_\sigma - \Theta \cdot j_{\bar{\sigma}})\,. \tag{4.4.10}$$

By observing (4.3.14) and (4.4.5), one finds

$$j_\sigma^+ = v_\sigma^+ p_\sigma - \frac{\partial}{\partial x} \cdot (\mathbf{D}_\sigma p_\sigma) \tag{4.4.11}$$

$$j_\sigma^- = v_\sigma^- p_\sigma \tag{4.4.12}$$

with the even and odd components $v_\sigma^\pm$ of the drift vector defined in the same way as (4.4.9, 10). One then obtains from (4.4.5)–(4.4.7) the set

$$\mathbf{D}_\sigma^- \equiv \tfrac{1}{2}(\mathbf{D}_\sigma - \boldsymbol{\Theta} \cdot \mathbf{D}_{\bar{\sigma}} \cdot \boldsymbol{\Theta}) = 0 \qquad \text{on the support of } p_\sigma \tag{4.4.13}$$

$$j_\sigma^+ = 0 \tag{4.4.14}$$

$$\frac{\partial}{\partial \boldsymbol{x}} \cdot j_\sigma^- = 0 \tag{4.4.15}$$

which are necessary and sufficient conditions for generalised detailed balance. A covariant formulation of these conditions has been discussed in ref. [67], and it can be shown that a transformation $\sigma \to \bar{\sigma}$, $\boldsymbol{x} \to \boldsymbol{\Theta} \cdot \boldsymbol{x}$ obeying the generalized detailed-balance relation (4.3.11) exists for any Fokker–Planck process [103]. This result has, however, not proved very useful, because the stationary distribution has to be known a priori in order to construct the transformation.

By applying the Fokker–Planck operator to the function $\boldsymbol{x}\, p_\sigma(\boldsymbol{x})$, we obtain with the help of (3.5.14) further the relation

$$\int \Gamma_\sigma(\boldsymbol{x}, \boldsymbol{y})\, \boldsymbol{y}\, p_\sigma(\boldsymbol{y})\, \mathrm{d}\boldsymbol{y} = [\boldsymbol{v}_\sigma^+(\boldsymbol{x}) - \boldsymbol{v}_\sigma^-(\boldsymbol{x})]\, p_\sigma(\boldsymbol{x})\,, \tag{4.4.16}$$

which will prove useful for the derivation of a fluctuation theorem (see section 5.2).

An important consequence follows in the case of nonsingular $\mathbf{D}_\sigma$. Then (4.4.14) leads to the "potential condition"

$$\frac{\partial}{\partial \boldsymbol{x}} \ln p_\sigma = \mathbf{D}_\sigma^{-1} \cdot \left\{ v_\sigma^+ - \left(\frac{\partial}{\partial \boldsymbol{x}} \cdot \mathbf{D}_\sigma \right) \right\} \tag{4.4.17}$$

which yields the stationary distribution

$$p_\sigma = Z_\sigma^{-1} \exp(-\Phi_\sigma) \tag{4.4.18a}$$

with a distribution potential Φ_σ determined by

$$\frac{\partial \Phi_\sigma}{\partial \boldsymbol{x}} = -\mathbf{D}_\sigma^{-1} \cdot \left\{ \boldsymbol{v}_\sigma^+ - \left(\frac{\partial}{\partial \boldsymbol{x}} \cdot \mathbf{D}_\sigma \right) \right\}. \tag{4.4.18b}$$

In the case of strict detailed balance, one has

$$\boldsymbol{v}_\sigma^- \equiv 0, \qquad \boldsymbol{v}_\sigma = \boldsymbol{v}_\sigma^+, \tag{4.4.19}$$

and the Fokker–Planck operator may be symmetrised by the transformation (4.3.21). It then becomes equivalent to a Schrödinger-like operator

$$I^{\text{symm}} = \frac{\partial}{\partial x} \cdot \mathbf{D} \cdot \frac{\partial}{\partial x} - \mathbf{V}(x) \tag{4.4.20}$$

with generally x-dependent anisotropic mass $\mathbf{m} = \frac{1}{2}\hbar^2 \mathbf{D}^{-1}$ and an effective potential

$$V(x) = \frac{1}{4}\left[v - \left(\frac{\partial}{\partial x} \cdot \mathbf{D}\right)\right] \cdot \mathbf{D}^{-1} \cdot \left[v - \left(\frac{\partial}{\partial x} \cdot \mathbf{D}\right)\right] + \frac{1}{2}\frac{\partial}{\partial x} \cdot \left[v - \left(\frac{\partial}{\partial x} \cdot \mathbf{D}\right)\right]. \tag{4.4.21}$$

Comparison with (4.4.19) shows that the effective Schrödinger potential $V(x)$ may be expressed in terms of the distribution potential $\Phi(x)$ by

$$V(x) = \frac{1}{4}\frac{\partial \Phi}{\partial x} \cdot \mathbf{D} \cdot \frac{\partial \Phi}{\partial x} - \frac{1}{2}\frac{\partial}{\partial x} \cdot \mathbf{D} \cdot \frac{\partial}{\partial x}\Phi. \tag{4.4.22}$$

The useful set of relations (4.4.13–15) with Θ denoting time-reversal of the state variables has first been obtained for the Fokker–Planck description of systems in thermodynamic equilibrium by Green [3]. For a general Fokker–Planck process, the relations have been given by van Kampen [104], Uhlhorn [105] and Stratonovich [106]. They have been rediscovered by Graham and Haken [107] and Risken [108], who also showed that the relations (4.4.13–15) are necessary and sufficient conditions for detailed balance of Fokker–Planck processes.

4.4.E1. Detailed balance of the Gauss–Markov process

The time-homogeneous n-component Gauss–Markov process is a Fokker–Planck process with (see (2.2.36, 37))

$$v_\sigma(x) = \dot{\boldsymbol{\rho}}_\sigma \cdot x + \dot{\boldsymbol{\alpha}}_\sigma; \qquad \mathbf{D}_\sigma = \tfrac{1}{2}\dot{\boldsymbol{\sigma}}_\sigma, \tag{4.4.23}$$

where we have dropped the subscript 0 for simplicity. The stationary distribution satisfies

$$\frac{\partial}{\partial x} \ln p_\sigma(x) = -\mathbf{s}_\sigma^{-1} \cdot (x - a_\sigma), \tag{4.4.24}$$

where a_σ and $\mathbf{s}_\sigma$ are related to $\dot{\boldsymbol{\sigma}}_\sigma$, $\dot{\boldsymbol{\rho}}_\sigma$ and $\dot{\boldsymbol{\alpha}}_\sigma$ by (1.3.62, 63). Therefore, the stationary probability current may be written

$$j_\sigma(x) = \boldsymbol{\Omega}_\sigma \cdot \partial p_\sigma(x)/\partial x \tag{4.4.25}$$

with the antisymmetric tensor

$$\boldsymbol{\Omega}_\sigma = -\dot{\boldsymbol{\rho}}_\sigma \cdot \mathbf{s}_\sigma - \tfrac{1}{2}\dot{\boldsymbol{\sigma}}_\sigma = -\boldsymbol{\Omega}_\sigma^\dagger. \tag{4.4.26}$$

In the presence of generalised detailed balance, the even and odd components of the probability current are given by

$$j_\sigma^\pm(x) = \boldsymbol{\Omega}_\pm \cdot \partial p_\sigma(x)/\partial x \tag{4.4.27}$$

where

$$\mathbf{\Omega}_{\pm} = \tfrac{1}{2}(\mathbf{\Omega}_{\sigma} \pm \mathbf{\Theta} \cdot \mathbf{\Omega}_{\bar{\sigma}} \cdot \mathbf{\Theta}), \tag{4.4.28}$$

and the conditions (4.4.13, 14) take the form

$$\dot{\boldsymbol{\sigma}}_{-} = 0, \qquad \dot{\boldsymbol{\sigma}}_{\sigma} = \dot{\boldsymbol{\sigma}}_{+} \tag{4.4.29}$$

$$\mathbf{\Omega}_{+} = 0, \qquad \mathbf{\Omega}_{\sigma} = \mathbf{\Omega}_{-}. \tag{4.4.30}$$

The third condition (4.4.15) is automatically satisfied on account of the antisymmetry of $\mathbf{\Omega}_{-}$.

From (4.4.30) and (4.4.26) one obtains

$$\dot{\boldsymbol{\sigma}}_{\sigma} = -2\dot{\boldsymbol{\rho}}_{+} \cdot \mathbf{s}_{\sigma} = -2\mathbf{s}_{\sigma} \cdot \dot{\boldsymbol{\rho}}_{+}^{\dagger} \tag{4.4.31}$$

which shows that $\dot{\boldsymbol{\rho}}_{+} \cdot \mathbf{s}$ and therefore also

$$\dot{\boldsymbol{\rho}}_{+} \cdot \dot{\boldsymbol{\sigma}}_{\sigma} = \dot{\boldsymbol{\sigma}}_{\sigma} \cdot \dot{\boldsymbol{\rho}}_{+}^{\dagger} \tag{4.4.32}$$

is symmetric. Further, $\mathbf{\Omega}_{\sigma}$ is given by

$$\mathbf{\Omega}_{\sigma} = -\dot{\boldsymbol{\rho}}_{-} \cdot \mathbf{s}_{\sigma} = +\mathbf{s}_{\sigma} \cdot \dot{\boldsymbol{\rho}}_{-}^{\dagger}, \tag{4.4.33}$$

which shows that $\dot{\boldsymbol{\rho}}_{-} \cdot \mathbf{s}_{\sigma}$ is antisymmetric, and

$$\operatorname{tr} \dot{\boldsymbol{\rho}}_{-} = 0. \tag{4.4.34}$$

It is interesting to note that any Gauss–Markov process satisfies generalised detailed balance with $\mathbf{\Theta} = \mathbf{1}$ and $\bar{\sigma}$ defined by

$$\dot{\boldsymbol{\sigma}}_{\bar{\sigma}} = \dot{\boldsymbol{\sigma}}_{\sigma} \tag{4.4.35}$$

$$\dot{\boldsymbol{\rho}}_{\bar{\sigma}} = \mathbf{s}_{\sigma} \cdot \dot{\boldsymbol{\rho}}_{\sigma}^{\dagger} \cdot \mathbf{s}_{\sigma}^{-1} \tag{4.4.36}$$

$$\dot{\boldsymbol{\alpha}}_{\bar{\sigma}} = -\dot{\boldsymbol{\rho}}_{\bar{\sigma}} \cdot \boldsymbol{a}_{\bar{\sigma}} \tag{4.4.37}$$

such that

$$\mathbf{\Omega}_{\bar{\sigma}} = -\mathbf{\Omega}_{\sigma}. \tag{4.4.38}$$

A vanishing $\mathbf{\Omega}_{\sigma}$ implies simple detailed balance with $\bar{\sigma} = \sigma$.

In the case of strict detailed balance (4.3.20), the Fokker–Planck operator (4.4.1a) may be symmetrised by the transformation (4.3.21). By comparison with (4.4.20, 21) one obtains (up to a minus sign) the Schrödinger operator

$$I^{\text{symm}} = \frac{\hbar^2}{2} \frac{\partial}{\partial \boldsymbol{x}} \cdot \mathbf{m}^{-1} \cdot \frac{\partial}{\partial \boldsymbol{x}} - V(\boldsymbol{x}) \tag{4.4.39}$$

$$V(x) = \tfrac{1}{2}(x-a)\cdot \mathbf{C}\cdot(x-a) + V_0 \tag{4.4.40}$$

of a multi-dimensional harmonic oscillator with mass tensor

$$\mathbf{m} = \hbar^2 \dot{\boldsymbol{\sigma}}_0^{-1}, \tag{4.4.41}$$

restoring-force tensor

$$\mathbf{C} = \dot{\boldsymbol{\rho}}_0^{\dagger}\cdot\dot{\boldsymbol{\sigma}}_0^{-1}\cdot\dot{\boldsymbol{\rho}}_0, \tag{4.4.42}$$

and a constant background potential

$$V_0 = \tfrac{1}{2}\mathrm{tr}\,\dot{\boldsymbol{\rho}}_0. \tag{4.4.43}$$

We restrict the further discussion to the case $\dot{\boldsymbol{\sigma}}_0$ positive-definite and $\dot{\boldsymbol{\rho}}_0$ a "stability matrix" (see (2.2.49)). If $\dot{\boldsymbol{\rho}}_0$ and $\dot{\boldsymbol{\sigma}}_0$ commute, we recover the example treated in section 3.2.E2. In the general case, the transformation

$$x = \dot{\boldsymbol{\sigma}}_0^{1/2}\cdot\zeta + a \tag{4.4.44}$$

diagonalizes the kinetic energy and yields

$$I^{\mathrm{symm}} = \frac{1}{2}\frac{\partial}{\partial\zeta}\cdot\frac{\partial}{\partial\zeta} - \frac{1}{2}\zeta\cdot\boldsymbol{\Lambda}^{\dagger}\cdot\boldsymbol{\Lambda}\cdot\zeta - V_0, \tag{4.4.45}$$

where the matrix $\boldsymbol{\Lambda}$ is given by

$$\boldsymbol{\Lambda} = \dot{\boldsymbol{\sigma}}_0^{-1/2}\cdot\dot{\boldsymbol{\rho}}_0\cdot\dot{\boldsymbol{\sigma}}_0^{1/2}. \tag{4.4.46}$$

By using eq. (4.4.31), this may be written in the form

$$\boldsymbol{\Lambda} = -\tfrac{1}{2}\dot{\boldsymbol{\sigma}}_0^{1/2}\cdot\mathbf{s}\cdot\boldsymbol{\sigma}_0^{1/2}, \tag{4.4.47}$$

which shows that $\boldsymbol{\Lambda}$ is Hermitian and negative definite, and the eigenfrequencies ω_i of the harmonic oscillator are given by the negative eigenvalues λ_i of $\boldsymbol{\Lambda}$. Further, by using (4.4.46) one finds for the background potential (4.4.43) the expression

$$V_0 = \tfrac{1}{2}\mathrm{tr}\,\boldsymbol{\Lambda} = \tfrac{1}{2}\sum_i \lambda_i < 0. \tag{4.4.48}$$

This shows that V_0 just compensates the zero-point energy of the harmonic oscillators, which is required to ensure the eigenvalue $\lambda_0 = 0$ of the master operator.

We have thus found that the spectrum of the master operator (4.4.39) is given by

$$\lambda_{\{n_i\}} = \sum_i n_i\lambda_i, \qquad n_i = 0, 1, 2, \ldots, \tag{4.4.49}$$

where λ_i are the eigenvalues of the operator $\boldsymbol{\Lambda}$ defined in (4.4.46).

5. Linear response theory for stochastic processes

The study of linear response of a system to external test forces has proved to be a very useful method for the investigation of the dynamics of systems in thermodynamic equilibrium [7, 109–112]. Apart from giving the response of the system to actual perturbations, the generalised susceptibility yields information about relaxation towards equilibrium, about normal modes and via the famous fluctuation-dissipation theorem [7, 27, 28] about the fluctuations of the unperturbed system, even in cases where experimental realization of the test forces may be difficult.

In this section, we develop the formalism to calculate the linear response of a Markov process to an arbitrary external test force. The case of non-Markov processes has been treated in ref. [30, 113]. We shall be especially interested in fluctuation theorems relating the susceptibility to correlations between fluctuations of the unperturbed system.

5.1. Linear response of a Markov process

We consider a stochastic process $\hat{x}(t)$ which differs from a given reference process $x(t)$ by a small perturbation. The time evolution of the perturbed process is governed by the master operator

$$\hat{\Gamma}(t) = \Gamma(t) + \Gamma'(t) \tag{5.1.1}$$

where $\Gamma(t)$ refers to the reference process. We explicitly assume that both the unperturbed and the perturbed process are of Markov character.

The perturbation $\Gamma'(t)$ represents the change of the transition probabilities by an externally controllable force $F(t)$ which we assume to be real. For the purpose of linear response it is sufficient to consider a linear coupling

$$\Gamma'(t) = F(t)\,\Omega(t) \tag{5.1.2}$$

described by an operator $\Omega(t)$ which for a nonstationary process will in general be time-dependent. The force $F(t)$ may be a mechanical, electric or magnetic force acting on the system, or may be of thermal or chemical origin, describing a change of the coupling to the external reservoirs. From eq. (2.3.5) applied to $\hat{\Gamma}(t)$ one obtains a condition for the kernel of the operator $\Omega(t)$,

$$\int \Omega(x, y; t)\,\mathrm{d}x = 0\,, \tag{5.1.3}$$

which guarantees conservation of probability normalization under the perturbation.

The master operator $\hat{\Gamma}(t)$ generates the perturbed propagator $\hat{R}(t|s)$ for which one obtains the Dyson-type equation

$$\hat{R}(t|t_0) = R(t|t_0) + \int_{t_0}^{t} R(t|s)\,\Gamma'(s)\,\hat{R}(s|t_0)\,\mathrm{d}s, \qquad t \geq t_0\,, \tag{5.1.4}$$

where $R(t|t_0)$ is the unperturbed propagator. The perturbation is assumed to be switched on after the system is prepared at time t_0 with initial distribution $p(t_0) = p_0$.

Up to linear terms in the force $F(t)$, the probability distribution $\hat{p}(t) = \hat{R}(t|t_0)p_0$ of the perturbed process is obtained by replacing $\hat{R}(s|t)$ on the r.h.s. of (5.1.4) by $R(s|t)$ and using (5.1.2) as

$$\hat{p}(t) = p(t) + \int_{t_0}^{t} R(t|s)\,\Omega(s)\,p(s)\,F(s)\,\mathrm{d}s\,. \tag{5.1.5}$$

The linear response of the statistical average of a stochastic variable $f(t)$ assumed to be real, to the force $F(t)$,

$$\begin{aligned}\langle \delta f(t)\rangle &= \langle f(t)\rangle_{\hat{p}(t)} - \langle f(t)\rangle_{p(t)} \\ &= \int_{t_0}^{\infty} \chi(t, s)\,F(s)\,\mathrm{d}s\end{aligned} \tag{5.1.6}$$

defines the *generalised susceptibility* $\chi(t, s)$.

From (5.1.5) one obtains

$$\chi(t, s) = \theta(t-s) \int\int f(xt)\,R(xt|ys)\,[\Omega(s)\,p(s)]_y\,\mathrm{d}x\,\mathrm{d}y\,, \tag{5.1.7}$$

where the unit-step function $\theta(t-s)$ guarantees the *causality requirement* (the integral in (5.1.6) may then be extended to ∞).

For a nonstationary process, the susceptibility $\chi(t_2, t_1)$ depends separately on two time instants t_1 and t_2. From an experimental point of view, $\chi(t_2, t_1)$ can be measured as the response at time t_2 to a δ-impulse at time t_1. Similarly, its double Fourier transform

$$\chi(\omega_2, \omega_1) = \int\int \chi(t_2, t_1)\exp[\mathrm{i}(\omega_2 t_2 - \omega_1 t_1)]\,\mathrm{d}t_2\,\mathrm{d}t_1 \tag{5.1.8}$$

can be measured as the response at frequency ω_2 to a unit-amplitude harmonic force at frequency ω_1.

The susceptibility $\chi(\omega_2, \omega_1)$ may be extended to complex frequencies z_2, z_1. From the causality requirement $\chi(t_2, t_1) = 0$ for $t_2 < t_1$, it follows that $\chi(z_2, z_1)$ is separately regular in the upper half-planes of both variables z_2 and z_1, and one obtains the spectral representations

$$\left.\begin{aligned}\chi(z_2, z_1) &= \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{+\infty} \frac{\chi(\omega', z_1)}{\omega' - z_2}\,\mathrm{d}\omega' \qquad (5.1.9\mathrm{a}) \\ &= \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{+\infty} \frac{\chi(z_2, \omega')}{z_1 - \omega}\,\mathrm{d}\omega' \qquad (5.1.9\mathrm{b})\end{aligned}\right\} \quad (\mathrm{Im}\,z_1, \mathrm{Im}\,z_2 > 0)\,.$$

On the real axes, this yields dispersion relations between real and imaginary parts of $\chi(\omega_2, \omega_1)$ in both frequency variables ω_2 and ω_1 separately [114],

$$\chi'(\omega_2, \omega_1) = \frac{1}{\pi} \fint_{-\infty}^{+\infty} \frac{\chi''(\omega', \omega_1)}{\omega' - \omega_2} \, d\omega' = \frac{1}{\pi} \fint_{-\infty}^{+\infty} \frac{\chi''(\omega_2, \omega')}{\omega_1 - \omega'} \, d\omega' \tag{5.1.10a}$$

$$\chi''(\omega_2, \omega_1) = -\frac{1}{\pi} \fint_{-\infty}^{+\infty} \frac{\chi'(\omega', \omega_1)}{\omega' - \omega_2} \, d\omega' = -\frac{1}{\pi} \fint_{-\infty}^{+\infty} \frac{\chi'(\omega_2, \omega')}{\omega_1 - \omega'} \, d\omega' \tag{5.1.10b}$$

where $\fint$ denotes the principal value of the integral.

For real $F(t)$ and $f(t)$, $\chi(t_2, t_1)$ is real, and one obtains the *reality condition*

$$\chi(-z_2^*, -z_1^*) = \chi^*(z_2, z_1) . \tag{5.1.11}$$

Thus, $\chi(z_2, z_1)$ is real for purely imaginary z_2, z_1. On the real axis, one has the symmetry relations

$$\chi'(-\omega_2, -\omega_1) = \chi'(\omega_2, \omega_1) \tag{5.1.12a}$$

$$\chi''(-\omega_2, -\omega_1) = -\chi''(\omega_2, \omega_1) . \tag{5.1.12b}$$

If the unperturbed process is strictly stationary, $R(t|s) = R(t-s)$, $p(t) = p_s$, the operator Ω is independent of time. If in addition the variable f does not explicitly depend on time, then the susceptibility becomes time-homogeneous,

$$\chi(s+\tau, s) \equiv \chi(\tau) = \theta(\tau) \int\int f(x) \, R(x\tau|y0) \, [\Omega p_s]_y \, dx \, dy , \tag{5.1.13}$$

and in Fourier space, one obtains a linear response only at the frequency of the driving force,

$$\chi(\omega, \omega') = \chi(\omega) \cdot 2\pi\delta(\omega - \omega') , \tag{5.1.14}$$

where

$$\chi(\omega) = \int_0^\infty \chi(\tau) \exp(i\omega\tau) \, d\tau . \tag{5.1.15}$$

The spectral representation (5.1.9) and the dispersion relations (5.1.10) then take the familiar form

$$\chi(z) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{\chi(\omega')}{\omega' - z} \, d\omega' \qquad (\mathrm{Im}\, z > 0) \tag{5.1.16}$$

and

$$\chi'(\omega) = \frac{1}{\pi} \fint_{-\infty}^{+\infty} \frac{\chi''(\omega')}{\omega' - \omega} \, d\omega' \tag{5.1.17a}$$

$$\chi''(\omega) = -\frac{1}{\pi} \oint_{-\infty}^{+\infty} \frac{\chi'(\omega')}{\omega' - \omega} \, \mathrm{d}\omega' , \tag{5.1.17b}$$

respectively, and for real F and f one has the reality conditions

$$\chi(-z^*) = \chi^*(z) \tag{5.1.18}$$

$$\chi'(-\omega) = \chi'(\omega), \qquad \chi''(-\omega) = -\chi''(\omega) . \tag{5.1.19}$$

Another important case is the response to a constant unit force which is switched off at time $t = 0$. This response, which describes the relaxation of the system back to its stationary state, is given by the *relaxation function*

$$\Phi(t) = \int_t^\infty \chi(\tau) \, \mathrm{d}\tau . \tag{5.1.20}$$

Its initial value is the static susceptibility

$$\Phi(t = 0) = \chi(\omega = 0) . \tag{5.1.21}$$

5.2. Fluctuation theorems

The form of eq. (5.1.7) suggests to introduce a stochastic variable $\vartheta(t)$ associated with the perturbation $\Gamma'(t) = F(t)\, \Omega(t)$ by the definition

$$\vartheta(xt)\, p(xt) = [\Omega(t)\, p(t)]_x . \tag{5.2.1}$$

The statistical average of $\vartheta(t)$ vanishes on account of eq. (5.1.3),

$$\langle \vartheta(t) \rangle = 0 , \tag{5.2.2}$$

i.e. $\vartheta(t)$ represents a fluctuation of the system. Therefore, the expression (5.1.7) for the susceptibility takes the form of a *fluctuation theorem* [114, 115]

$$\begin{aligned} \chi(t, s) &= \theta(t - s) \langle f(t)\, \vartheta(s) \rangle \\ &= \theta(t - s) \langle \varphi(t)\, \vartheta(s) \rangle \equiv \theta(t - s)\, S_{\varphi\vartheta}(t, s) , \end{aligned} \tag{5.2.3}$$

connecting the response to an external perturbation with the unperturbed correlation between the fluctuations $\varphi(t) = f(t) - \langle f(t) \rangle$ and $\vartheta(t)$.

We now restrict the discussion to strictly stationary processes and to variables f which do not depend explicitly on time, such that the susceptibility becomes time-homogeneous,

$$\chi(\tau) = \theta(\tau) \langle \varphi(\tau)\, \vartheta(0) \rangle \equiv \theta(\tau)\, S_{\varphi\vartheta}(\tau) . \tag{5.2.4}$$

In this case one may derive an alternative fluctuation theorem which resembles more closely the fluctuation-dissipation theorem for equilibrium systems [7, 27, 28]. With the perturbed process described by the stochastic operator $\hat{\Gamma}(t) = \Gamma + F(t)\,\Omega$ we associate an *accompanying distribution* ("begleitende Verteilung") $p_a(F(t))$ defined by

$$[\Gamma + F(t)\Omega]p_a = 0\,. \tag{5.2.5}$$

Physically, $p_a(F(t))$ represents the stationary distribution in a system in which $F(t)$ is frozen at its instantaneous value. Note that p_a depends on time only indirectly via $F(t)$.

The linear response δp_a to $F(t)$ is determined by

$$\Gamma\,\delta p_a + \Omega p_s\,F(t) = 0\,. \tag{5.2.6}$$

We define a variable ψ associated with the perturbation $\Gamma'(t) = \Omega\,F(t)$ by the relation

$$\delta p_a(x;\,F(t)) = \psi(x)\,p_s(x)\,F(t)\,, \tag{5.2.7}$$

such that

$$[\Omega p_s]_x = -\int \Gamma(x,\,z)\,\psi(z)\,p_s(z)\,\mathrm{d}z\,. \tag{5.2.8}$$

It is not necessary to assume that the accompanying distribution is normalizable, but we will assume that $p_a(F=0) = p_s$ and that $\delta N = \int \delta p_a(x;\,F)\,\mathrm{d}x$ exists. The value of δN may then be made equal to zero by a change of normalization $p_a \to p_a/(1+\delta N)$. For this normalization, $\psi(x)$ again represents a fluctuation of the system,

$$\langle\psi\rangle = 0\,, \tag{5.2.9}$$

and the expression (5.1.13) may be written

$$\chi(\tau) = -\theta(\tau)\int\int\int f(x)\,R(x\tau|y0)\,\Gamma(y,\,z)\,\psi(z)\,p_s(z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,. \tag{5.2.10}$$

By using eqs. (2.2.10) and (5.2.9), this may be transformed into

$$\begin{aligned}\chi(\tau) &= -\theta(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau}\int\int \varphi(x)\,R(x\tau|z0)\,\psi(z)\,p_s(z)\,\mathrm{d}x\,\mathrm{d}z \\ &= -\theta(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau}\langle\varphi(\tau)\,\psi(0)\rangle \equiv -\theta(\tau)\frac{\mathrm{d}S_{\varphi\psi}(\tau)}{\mathrm{d}\tau}\,,\end{aligned} \tag{5.2.11}$$

which again connects the linear response with an unperturbed correlation between the fluctuations $\varphi = f - \langle f\rangle$ and ψ. However, whereas the variable ϑ is given explicitly by eq. (5.2.1), the variable ψ is given only implicitly as the solution of (5.2.8), or equivalently, if the accompanying distribution $p_a(F)$ is

assumed to be known as function of F, by the derivative

$$\psi(x)\, p_s(x) = \partial p_a(x; F)/\partial F|_{F=0}\,. \tag{5.2.12}$$

With the help of the spectral decomposition (3.2.12) of the conditional probability, we obtain a special representation of the susceptibility tensor. We assume that the eigenvalue $\lambda_0 = 0$ is nondegenerate, i.e. the stationary distribution p_s is unique, and find in analogy to (3.2.16, 17)

$$\chi(\tau) = \theta(\tau) \sum_{n\geq 1} g_n^{(\varphi)} h_n^{(\vartheta)*} \exp(\lambda_n \tau) \tag{5.2.13a}$$

$$= -\theta(\tau) \sum_{n} \lambda_n g_n^{(\varphi)} h_n^{(\psi)*} \exp(\lambda_n \tau)\,, \tag{5.2.13b}$$

or in Fourier space

$$\chi(\omega) = -\sum_{n\geq 1} \frac{1}{\lambda_n + i\omega}\, g_n^{(\varphi)} h_n^{(\vartheta)*} \tag{5.2.14a}$$

$$= \sum_{n} \frac{\lambda_n}{\lambda_n + i\omega}\, g_n^{(\varphi)} h_n^{(\psi)*}\,, \tag{5.2.14b}$$

where the g_n and h_n are defined as in eq. (3.2.14, 15) in terms of the eigenfunctions φ_n, ψ_n of the master operator,*

$$g_n^{(\varphi)} = \int \varphi(x)\, \psi_n(x)\, dx \tag{5.2.15a}$$

$$h_n^{(\vartheta)} = \langle \vartheta \varphi_n \rangle \tag{5.2.15b}$$

$$h_n^{(\psi)} = \langle \psi \varphi_n \rangle\,. \tag{5.2.15c}$$

We illustrate these concepts by a few specific situations. A classification of fluctuation theorems for Markov processes is given in ref. [115].

1. Isolated system with Liouville dynamics
Here, the time evolution is governed by the Liouville generator

$$\Gamma = \{H(x), \quad\}\,, \tag{5.2.16}$$

where $H(x)$ is the Hamiltonian, and $\{\ \}$ are the Poisson brackets. The perturbation is described by a Hamiltonian

$$H'(x) = -F(t)\, g(x)\,, \tag{5.2.17}$$

* The left and right eigenfunctions φ_n, ψ_n of the master operator should not be confused with the state functions $\varphi = f - \langle f \rangle$ and ψ.

i.e. the operator Ω has the form

$$\Omega = -\{g(x), \quad\}. \tag{5.2.18}$$

For a canonical stationary distribution

$$p_s(x) = Z^{-1} \exp[-H(x)/kT], \tag{5.2.19}$$

one then finds from eq. (5.2.1)

$$\vartheta(x) = \{g(x), H(x)\}/kT \equiv \dot{g}(x)/kT, \tag{5.2.20}$$

and from eq. (5.2.8)

$$\psi(x) = g(x)/kT, \tag{5.2.21}$$

and therefore from both eqs. (5.2.4) and (5.2.11)

$$\chi(\tau) = -\frac{\theta(\tau)}{kT}\frac{\mathrm{d}}{\mathrm{d}\tau}\langle\varphi(\tau)\, g(0)\rangle = -\frac{\theta(\tau)}{kT}\frac{\mathrm{d}S_{\varphi g}(\tau)}{\mathrm{d}\tau}, \tag{5.2.22}$$

which is the classical *fluctuation-dissipation theorem* in the time domain [7].

It should be noted, however, that in this case of an isolated system not in continuous contact with a heat bath, the usual derivation of linear response amounts to assuming linear perturbations of the system trajectories, an assumption which is valid only for unphysically small values of the external force, as has been emphasized by van Kampen [116, 117].

2. *Canonical form of accompanying distribution*
If the solution of eq. (5.2.5) is of the form

$$p_a(x; F) = [Z(F)]^{-1} \exp[-\Phi(x) + Fh(x)], \tag{5.2.23}$$

i.e.

$$\delta p_a(x; F) = F \cdot [h(x) - \langle h\rangle]\, p_s(x), \tag{5.2.24}$$

then one sees by comparison with (5.2.7) that

$$\psi(x) = h(x) - \langle h\rangle \tag{5.2.25}$$

and therefore

$$\chi(\tau) = -\theta(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau}\langle\varphi(\tau)\, h(0)\rangle \equiv -\theta(\tau)\frac{\mathrm{d}S_{\varphi h}(\tau)}{\mathrm{d}\tau}. \tag{5.2.26}$$

3. *Gradient perturbation*
An important case is the coupling of a vector force $\boldsymbol{F}$ to the gradient of the probability distribution,

$$[\Gamma'(t)\, p(t)]_x = -\kappa\, \boldsymbol{F}(t) \cdot \partial p(xt)/\partial \boldsymbol{x}\,, \tag{5.2.27}$$

i.e.

$$\Omega = -\kappa\, \partial/\partial x\,. \tag{5.2.28}$$

One finds from eq. (5.2.1) [114]

$$\vartheta(xt) = -\kappa \frac{\partial}{\partial x} \ln p_s(xt)\,. \tag{5.2.29}$$

For a stationary Fokker–Planck process obeying generalized detailed-balance symmetry, with a constant nonsingular diffusion matrix, one finds from eq. (4.4.17)

$$\boldsymbol{\vartheta}(\boldsymbol{x}) = -\kappa\, \mathbf{D}^{-1} \cdot \boldsymbol{v}^{+}(\boldsymbol{x})\,, \tag{5.2.30}$$

where v^+ is the even part of the drift vector. In the case of strict detailed balance (4.4.19), one obtains by using eq. (4.4.16)

$$\vartheta(x)\, p_s(x) = -\kappa\, \mathbf{D}^{-1} \cdot \int \Gamma(x, y)\, y\, p_s(y)\, \mathrm{d}y\,, \tag{5.2.31}$$

whence by comparison with (5.2.8)

$$\psi(x) = \kappa\, \mathbf{D}^{-1} \cdot \xi\,. \tag{5.2.32}$$

For the response of the state vector $\boldsymbol{x}$, one thus finds the fluctuation theorem [118]

$$\chi(\tau) = -\theta(\tau)\, \kappa\, \mathbf{D}^{-1} \cdot \frac{\mathrm{d}}{\mathrm{d}\tau} \langle \xi(\tau)\, \xi(0) \rangle \equiv -\theta(\tau)\, \kappa\, \mathbf{D}^{-1} \cdot \frac{\mathrm{d}\mathbf{S}(\tau)}{\mathrm{d}\tau}\,. \tag{5.2.33}$$

This may be generalized to the case of an odd drift vector $\boldsymbol{v}^-$ related linearly to the even drift vector $\boldsymbol{v}^+$ [115].

5.2.*E*1. *Linear response of the two-state Markov process*
A general perturbation of the two-state process has the form

$$\Gamma'(t) = F_1(t) \begin{pmatrix} -1 & 0 \\ 1 & 0 \end{pmatrix} + F_2(t) \begin{pmatrix} 0 & 1 \\ 0 & -1 \end{pmatrix} = F_1(t)\, \Omega_1 + F_2(t)\, \Omega_2 \tag{5.2.34}$$

where

$$\Omega_1(x, y) = -\tfrac{1}{2}x(1+y), \qquad \Omega_2(x, y) = +\tfrac{1}{2}x(1-y)\,. \tag{5.2.35a}$$

Here, F_1 and F_2 have the significance of a change of the transition probabilities w_{21} and w_{12} respectively (see (2.2.21)). The operators Ω_1, Ω_2 may be expressed in terms of the Pauli matrices $\sigma_{1,2,3}$ (see (2.2.19)) as

$$\Omega_2 = -\tfrac{1}{2}(\mathbb{1} - \sigma_1 + \mathrm{i}\sigma_2 + \sigma_3), \qquad \Omega_2 = -\tfrac{1}{2}(\mathbb{1} - \sigma_1 - \mathrm{i}\sigma_2 - \sigma_3)\,. \tag{5.2.35b}$$

The functions $\vartheta_1(x)$, $\vartheta_2(x)$ defined by (5.2.1) are found by using the representation (1.1.18) of the unperturbed distribution $p(x, t)$ to have the form

$$\vartheta_1(x, t) = -\frac{\xi}{1-a(t)}, \qquad \vartheta_2(x, t) = +\frac{\xi}{1+a(t)}, \tag{5.2.36}$$

where $\xi = x - a$. The response of the state variable x to the forces $F_1(t)$, $F_2(t)$ is obtained from (5.2.3) in terms of the auto-covariance $s(t_2, t_1) = \langle \xi(t_2)\, \xi(t_1) \rangle$ as

$$\chi_1(t_2, t_1) = -\frac{s(t_2, t_1)}{1-a(t_1)}\,\theta(t_2 - t_1) \tag{5.2.37a}$$

$$\chi_2(t_2, t_1) = +\frac{s(t_2, t_1)}{1+a(t_1)}\,\theta(t_2 - t_1)\,. \tag{5.2.37b}$$

By using eqs. (1.3.28) and (1.3.22) this may be written in the form

$$\chi_1(t_2, t_1) = -[1 + a(t_1)]\,\rho(t_2, t_1)\,\theta(t_2 - t_1) \tag{5.2.38a}$$

$$\chi_2(t_2, t_1) = +[1 - a(t_1)]\,\rho(t_2, t_1)\,\theta(t_2 - t_1)\,. \tag{5.2.38b}$$

For a stationary process, we could alternatively have started from the accompanying distribution

$$p_{\mathrm{a}}(x; F) = \tfrac{1}{2}[1 + \hat{a}(F)\, x]\,, \tag{5.2.39}$$

where

$$\hat{a}(F) = \frac{\dot{\rho}_0 a - F_2 + F_1}{1 - F_2 - F_1}\,. \tag{5.2.40}$$

The functions $\psi_1(x)$, $\psi_2(x)$ defined by eq. (5.2.7) are found to have the form

$$\psi_1(x) = +\frac{1}{\dot{\rho}_0}\frac{\xi}{1-a}, \qquad \psi_2(x) = -\frac{1}{\dot{\rho}_0}\frac{\xi}{1+a}, \tag{5.2.41}$$

and eq. (5.2.11) yields the response

$$\chi_1(\tau) = -\frac{1}{1-a}\,\frac{\theta(\tau)}{\dot{\rho}_0}\,\frac{\mathrm{d}s(\tau)}{\mathrm{d}\tau} \tag{5.2.42a}$$

$$\chi_2(\tau) = +\frac{1}{1+a}\frac{\theta(\tau)}{\dot{\rho}_0}\frac{\mathrm{d}s(\tau)}{\mathrm{d}\tau}. \tag{5.2.42b}$$

By using eqs. (1.3.28), (1.3.22) and (2.2.28), this may be written

$$\chi_1(\tau) = -(1+a)\,\theta(\tau)\exp(\dot{\rho}_0\tau) \tag{5.2.43a}$$

$$\chi_2(\tau) = +(1-a)\,\theta(\tau)\exp(\dot{\rho}_0\tau), \tag{5.2.43b}$$

which agrees with (5.2.38a, b) for a stationary process. Fourier transformation yields the spectral representation

$$\chi_1(\omega) = +\frac{1+a}{\dot{\rho}_0 + \mathrm{i}\omega} \tag{5.2.44a}$$

$$\chi_2(\omega) = -\frac{1-a}{\dot{\rho}_0 + \mathrm{i}\omega}. \tag{5.2.44b}$$

We obtain a pure relaxation with relaxation frequency $\dot{\rho}_0$.

Instead of the forces F_1 and F_2 representing perturbations of the transition rates w_{21} and w_{12} we could have considered perturbations F_ρ, F_α of the quantities $\dot{\rho}_0$, $\dot{\alpha}_0$ determining the generator (2.2.17) of the process. On account of eq. (2.2.21), the two sets are related by

$$F_\rho = -F_1 - F_2, \qquad F_\alpha = -F_1 + F_2, \tag{5.2.45}$$

and the response to F_ρ, F_α is given by

$$\chi_\rho(t_2, t_1) = -\tfrac{1}{2}(\chi_1 + \chi_2) = \rho(t_2, t_1)\, a(t_1)\theta(t_2 - t_1) \tag{5.2.46a}$$

$$\chi_\alpha(t_2, t_1) = -\tfrac{1}{2}(\chi_1 - \chi_2) = \rho(t_2, t_1)\,\theta(t_2 - t_1). \tag{5.2.46b}$$

5.2.E2. Linear response of the Gauss–Markov process

We consider a state-independent perturbation of the drift,

$$\hat{v}(xt) = v(xt) + F(t). \tag{5.2.47}$$

Eq. (2.2.33) shows that the perturbation of the master operator is represented by the gradient operator

$$\Omega = -\partial/\partial x. \tag{5.2.48}$$

The functions $\vartheta_1(x)$, $\vartheta_2(x)$ defined by (5.2.1) are found by using the representation (1.1.18) of the distribution $p(xt)$ as

$$\vartheta(xt) = [\mathbf{s}(t)]^{-1} \cdot \xi, \tag{5.2.49}$$

where $\xi = x - a(t)$. The response tensor of the state variable x is found from eq. (5.2.3) in the form

$$\boldsymbol{\chi}(t_2, t_1) = \mathbf{s}(t_2, t_1) \cdot [\mathbf{s}(t_1)]^{-1}\, \theta(t_2 - t_1)\,. \tag{5.2.50}$$

By using eq. (1.3.47), this may be written

$$\boldsymbol{\chi}(t_2, t_1) = \boldsymbol{\rho}(t_2, t_1)\, \theta(t_2 - t_1)\,. \tag{5.2.51}$$

For a stationary process, we could have started alternatively from the accompanying distribution

$$p_a(\boldsymbol{x}; \boldsymbol{F}) = p_s(\boldsymbol{x}; \boldsymbol{a} - \dot{\boldsymbol{\rho}}_0^{-1} \cdot \boldsymbol{F})\,. \tag{5.2.52}$$

The function $\boldsymbol{\psi}(\boldsymbol{x})$ defined by eq. (5.2.7) is found to have the form

$$\boldsymbol{\psi}(\boldsymbol{x}) = -\boldsymbol{\xi} \cdot \mathbf{s}^{-1} \cdot \dot{\boldsymbol{\rho}}_0^{-1}\,, \tag{5.2.53}$$

and eq. (5.2.11) yields the response tensor

$$\boldsymbol{\chi}(\tau) = \theta(\tau) \frac{\mathrm{d}}{\mathrm{d}\tau} \mathbf{s}(\tau) \cdot \mathbf{s}^{-1} \cdot \dot{\boldsymbol{\rho}}_0^{-1}\,. \tag{5.2.54}$$

By using eqs. (1.3.47) and (2.2.46), this may be written

$$\boldsymbol{\chi}(\tau) = \theta(\tau) \exp(\dot{\boldsymbol{\rho}}_0 \tau)\,, \tag{5.2.55}$$

which agrees with (5.2.51) for a stationary process.

This result shows that one obtains a superposition of relaxation processes with relaxation frequencies given by the eigenvalues of $-\dot{\boldsymbol{\rho}}_0$.

5.3. Sum rules and continued fraction expansion

The frequency moments of the dynamic susceptibility $\chi(\omega)$ can be expressed in terms of equal-time correlation functions. Such relations are called *sum rules.*

From the Fourier inversion of eq. (5.1.15) it follows that the frequency moments $\chi^{(k)}$ of $\chi(\omega)$ are given by the time derivatives of $\chi(\tau)$ at $\tau = 0^+$,

$$\chi^{(k)} \equiv \frac{1}{2\pi} \int_{-\infty}^{+\infty} (-\mathrm{i}\omega)^k \chi(\omega)\, \mathrm{d}\omega = \left. \frac{\mathrm{d}^k \chi(\tau)}{\mathrm{d}\tau^k} \right|_{\tau = 0^+} \tag{5.3.1}$$

as long as both sides exist. If the even and odd parts of $\chi(\omega)$ vary for $\omega \to \pm\infty$ as $\omega^{-(n_e+1)}$ and $\omega^{-(n_o+1)}$, respectively, then the l.h. side exists only for k even and $< n_e$ or k odd and $< n_o$, whereas the r.h. side may exist for any k.

The time derivatives of $\chi(\tau)$ can be found by differentiating the fluctuation theorems (5.2.4) or (5.2.11). From the forward equation (2.2.4) we find

$$\left. \frac{\mathrm{d}^k R(\tau|0)}{\mathrm{d}\tau^k} \right|_{\tau = 0^+} = \Gamma^k; \qquad \Gamma^0 \equiv 1\,, \tag{5.3.2}$$

where Γ^k is the k-fold iterated propagator. We thus obtain the sum rules ($k < n_e, n_o$)

$$\chi^{(k)} = \langle \varphi \vartheta_k \rangle \equiv S_{\varphi\vartheta_k} \tag{5.3.3a}$$

$$= -\langle \varphi \psi_{k+1} \rangle \equiv -S_{\varphi\psi_{k+1}}, \tag{5.3.3b}$$

where ϑ_k and ψ_k are defined by

$$\vartheta_k(x)\, p_s(x) = \int \Gamma^k(x, y)\, \vartheta(y)\, p_s(y)\, \mathrm{d}y \tag{5.3.4a}$$

$$\psi_k(x)\, p_s(x) = \int \Gamma^k(x, y)\, \psi(y)\, p_s(y)\, \mathrm{d}y, \tag{5.3.4b}$$

respectively.

It is of practical interest to express the dynamic susceptibility $\chi(\omega)$ in terms of equal-time correlation functions. We assume that $\chi(\tau)$ has a convergent Taylor expansion at $\tau = 0^+$,

$$\psi(\tau) = \theta(\tau) \sum_{k=0}^{\infty} \frac{1}{k!} \chi^{(k)} \tau^k. \tag{5.3.5}$$

Substituting this series in eq. (5.1.15) and observing $\int_0^\infty \tau^k \exp(\mathrm{i}\omega\tau)\, \mathrm{d}\tau = k!/(-\mathrm{i}\omega)^{k+1}$ yields an expansion of $\chi(\omega)$ in $1/\omega$,

$$\chi(\omega) = \sum_{k=0}^{\infty} \chi^{(k)}/(-\mathrm{i}\omega)^{k+1}, \tag{5.3.6}$$

with coefficients given by eq. (5.3.3). This series, which will in general be only semiconvergent, may be written in the form of continued fraction expansions

$$\chi(\omega) = \frac{c_1}{-\mathrm{i}\omega +} \; \frac{c_2}{1 +} \; \frac{c_3}{-\mathrm{i}\omega +} \cdots \tag{5.3.7a}$$

$$= \frac{b_1}{-\mathrm{i}\omega - a_1 +} \; \frac{b_2}{-\mathrm{i}\omega - a_2 +} \cdots \tag{5.3.7b}$$

which usually show fast convergence. The coefficients c_n, a_n and b_n are given in terms of the determinants

$$A_0 = 1, \qquad A_k = \det \begin{pmatrix} \chi^{(0)} & \cdots & \chi^{(k-1)} \\ \vdots & & \vdots \\ \chi^{(k-1)} & \cdots & \chi^{(2k-2)} \end{pmatrix} \quad (k \geq 1), \tag{5.3.8a}$$

and

$$B_1 = 1, \qquad B_k = \det \begin{pmatrix} \chi^{(1)} & \cdots & \chi^{(k-1)} \\ \vdots & & \vdots \\ \chi^{(k-1)} & \cdots & \chi^{(2k-3)} \end{pmatrix} \qquad (k \geq 2) \tag{5.3.8b}$$

as

$$c_1 = A_1, \qquad c_{2k} = -\frac{A_{k-1}B_{k+1}}{A_k B_k}, \qquad c_{2k+1} = -\frac{A_{k+1}B_k}{A_k B_{k+1}}, \tag{5.3.9}$$

and

$$\begin{aligned} &b_1 = c_1, \qquad a_1 = -c_2 \\ &b_{k+1} = -c_{2k}c_{2k+1}, \qquad a_{k+1} = -(c_{2k+1} + c_{2k+2}). \end{aligned} \tag{5.3.10}$$

For the calculation of high-order coefficients a convenient recursive algorithm has been developed [115, 119].

6. Specific systems

In the following, we discuss the stochastic behaviour of a number of specific systems. These may serve to demonstrate the application of the general concepts developed in the previous sections to problems of physical interest. In addition, the cases considered are intended to elucidate some aspects which have not been treated in the general theory. Of major interest is the problem of *phenomenological modelling*, i.e. of constructing a stochastic model of a macroscopic system, based on its phenomenological laws of motion, without recourse to the underlying microdynamics. Another problem discussed for the various cases is the *size scaling*, i.e. the dependence of the fluctuation properties on the size of the system [48, 49]. This is of particular importance in the case of systems which in the absence of fluctuations would show instabilities and multi-stable behaviour.

6.1. Brownian motion in a potential

Brownian motion has played an important role in the development of the theory of stochastic processes [1, 2, 7, 13, 18, 120, 121]. It has found application as a model for a variety of physical systems [1, 5, 42, 122–128]. In the following we consider a single Brownian particle of mass m in an external potential $U(x)$, interacting with a thermal environment, a heat bath at temperature T. The interaction with the heat bath gives rise to friction described by a constant friction coefficient $\gamma > 0$, and to fluctuating forces described by Gaussian white noise. We then have for position x and velocity u the system of SDE's (see section 2.4)

$$\begin{aligned} \mathrm{d}x &= u\,\mathrm{d}t \\ \mathrm{d}u &= -\left(\frac{1}{m}\frac{\partial U(x)}{\partial x} + \gamma u\right)\mathrm{d}t + b\,\mathrm{d}w(t) \end{aligned} \tag{6.1.1}$$

with $b = \text{const.}$, which is equivalent to the Fokker–Planck equation

$$\frac{\partial p}{\partial t} = -u\frac{\partial p}{\partial x} + \frac{\partial}{\partial u}\left[\left(\frac{1}{m}\frac{\partial U}{\partial x} + \gamma u\right)p\right] + \tfrac{1}{2}b^2\frac{\partial^2 p}{\partial u^2}. \tag{6.1.2}$$

In the case of a confining potential, $U(x) \to \infty$ for $x \to \pm\infty$, the stationary state is the thermal equilibrium state given by the Boltzmann distribution

$$p_s(x, u) = Z^{-1}\exp[-(\tfrac{1}{2}mu^2 + U(x))/kT]. \tag{6.1.3}$$

In order that this is compatible with the Fokker–Planck equation, the friction constant γ and the velocity-diffusion coefficient $D_u = \frac{1}{2}b^2$ must satisfy the Einstein relation

$$D_u = kT\gamma/m. \tag{6.1.4}$$

It may further be verified that the process satisfies the detailed-balance conditions (4.4.13–15) with a nonvanishing odd drift vector

$$v^-(x, u) = \left(u; -\frac{1}{m}\frac{\partial U}{\partial x}\right). \tag{6.1.5}$$

Therefore, the Fokker–Planck operator will in general have complex eigenvalues.

In the case of a driven system with a non vanishing stationary particle current, e.g. for $U(x) = U_p(x) - Fx$, U_p periodic or constant, with finite driving force F, there does not exist a universal form like (6.1.3) for the stationary distribution. It is not even certain that the ansatz (6.1.1) with b = constant is justified in this case.

In the case of strong damping, adiabatic elimination of the momentum leads to the Langevin equation for the position

$$\mathrm{d}x = -\frac{1}{m\gamma}\frac{\partial U}{\partial x}\mathrm{d}t + \frac{b}{\gamma}\mathrm{d}w(t), \tag{6.1.6}$$

which is equivalent to the *Smoluchowski equation*

$$\frac{\partial p}{\partial t} = \frac{1}{m\gamma}\frac{\partial}{\partial x}\left(\frac{\partial U}{\partial x}p\right) + D_x\frac{\partial^2 p}{\partial x^2} \tag{6.1.7}$$

with position-diffusion constant

$$D_x = \frac{1}{\gamma^2}D_u = \frac{kT}{m\gamma}. \tag{6.1.8}$$

It has to be noted that the validity of this Smoluchowski approximation depends on a condition depending both on the damping constant γ and on the gradient $\partial U/\partial x$ of the potential [1, 42, 129, 130].*

In the following, we calculate the linear response of an equilibrium system to an infinitesimal driving

* Eq. (6.1.7) is a good approximation for times long compared to γ^{-1} and if on the length scale $l = (kT/m\gamma^2)^{1/2}$ neither the potential nor the force vary appreciably; i.e., $l \cdot \partial U/\partial x \ll kT$, $l \cdot \partial^2 U/\partial x^2 \ll \partial U/\partial x$.

force $F(t)$. The perturbed system is described by a potential

$$\hat{U}(x, t) = U(x) - xF(t), \tag{6.1.9}$$

giving rise to a gradient-type perturbation

$$\Omega = -\frac{1}{m}\frac{\partial}{\partial u}$$

of the master operator. The linear response of the velocity variable, i.e. the *mobility* of the particle, is obtained from eqs. (5.2.4, 29) and (6.1.3) as

$$\chi_u(\tau) = \frac{\theta(\tau)}{kT}\langle u(\tau)\, u(0)\rangle \equiv \frac{\theta(\tau)}{kT} S_{uu}(\tau). \tag{6.1.10}$$

We have thus found the well-known result that the mobility is given by the velocity-autocorrelation function.

The linear response of the position variable, i.e. the ordinary *susceptibility* of the particle in the potential $U(x)$, is given by

$$\chi_x(\tau) = \frac{\theta(\tau)}{kT}\langle x(\tau)\, u(0)\rangle \equiv \frac{\theta(\tau)}{kT} S_{xu}(\tau), \tag{6.1.11}$$

which is equivalent to the usual form of the fluctuation theorem

$$\chi_x(\tau) = -\frac{\theta(\tau)}{kT}\frac{\mathrm{d}}{\mathrm{d}\tau}\langle x(\tau)\, x(0)\rangle \equiv -\frac{\theta(\tau)}{kT}\frac{\mathrm{d}S_{xx}(\tau)}{\mathrm{d}\tau}. \tag{6.1.12}$$

The two response functions χ_u and χ_x are obviously related by

$$\chi_u(\tau) = \mathrm{d}\chi_x(\tau)/\mathrm{d}\tau \tag{6.1.13}$$

$$\chi_u(\omega) = -\mathrm{i}\omega\chi_x(\omega) \tag{6.1.14}$$

in the time and frequency domain, respectively.

We now discuss the qualitative behaviour of the response for $\omega \to 0$:

– If $U(x)$ increases more strongly than linear,

$$U(x)/|x| \to \infty \text{ for } x \to \pm\infty,$$

then the perturbed potential $\hat{U}(x) = U(x) - Fx$ is still confining. Thus, a static force cannot give rise to a stationary current in any order of F, but will induce a finite displacement of the average position from its equilibrium value $\langle x\rangle = 0$. In linear response,

$$\left.\begin{array}{l}\chi_x(\omega) \to \chi_x^{(s)} \text{ finite} \\ \chi_u(\omega) \sim -\mathrm{i}\omega\chi_x^{(s)} \to 0\end{array}\right\} \quad \text{for } \omega \to 0. \tag{6.1.15}$$

For the simple example of a harmonic oscillator,

$$U(x) = \tfrac{1}{2} m\omega_0^2 x^2 , \tag{6.1.16}$$

one obtains explicitly (see ref. [2])

$$\left.\begin{aligned} \chi_x(\omega) &= \frac{1}{m(\omega_0^2 - \omega^2 - \mathrm{i}\gamma\omega)} \\ \chi_u(\omega) &= \frac{-\mathrm{i}\omega}{m(\omega_0^2 - \omega^2 - \mathrm{i}\gamma\omega)} \end{aligned}\right\} \quad \text{for all } \omega , \tag{6.1.17}$$

which is identical to the deterministic result. Of greater interest is the case of a particle in a multiwell potential, because of the conflict between deterministic multistability and stochastic asymptotic stability. We refer to section 6.3 where we discuss a problem equivalent to Brownian motion in a double-well potential.

– If $U(x)$ increases less strongly than linear,

$$U(x)/|x| \to 0 \qquad \text{for } x \to \pm\infty ,$$

then the perturbed potential $\hat{U}(x) = U(x) - Fx$ is no longer confining, and a static force will give rise to a nonvanishing current, while the average position will get displaced an infinite amount. However, both the position x_m and the value $U_m = U(x_m)$ of the potential maximum go to infinity when $F \to 0$ (e.g. if $U(x) \sim x^\alpha$ $(0 < \alpha < 1)$ then $x_m \sim F^{-1/(1-\alpha)}$ and $U_m \sim F^{-\alpha/(1-\alpha)}$). Therefore, the current vanishes exponentially when $F \to 0$, and the mobility is still zero:

$$\left.\begin{aligned} \chi_x(\omega) &\to \infty \\ \chi_u(\omega) &\to 0 \end{aligned}\right\} \quad \text{for } \omega \to 0 . \tag{6.1.18}$$

We thus expect an algebraic singularity at $\omega = 0$,

$$\left.\begin{aligned} \chi_x(\omega) &\sim \omega^{-\nu} \\ \chi_u(\omega) &\sim \omega^{1-\nu} \end{aligned}\right\} \quad 0 < \nu < 1 . \tag{6.1.19}$$

– If $U(x)$ is not confining, then no normalizable stationary distribution exists on the infinite interval. The case of a periodic or constant potential may still be treated by using the Fokker–Planck equation (6.1.2) and the equilibrium distribution (6.1.3) with periodic boundary condition.* In this case, one expects a finite static mobility $\chi_u^{(s)} = \chi_u(\omega = 0)$ and a diverging static susceptibility, i.e.

$$\left.\begin{aligned} \chi_u(\omega) &\to \chi_u^{(s)} \\ \chi_x(\omega) &\to \mathrm{i}\omega^{-1} \chi_u^{(s)} \to \infty \end{aligned}\right\} \quad \text{for } \omega \to 0 . \tag{6.1.20}$$

The position coordinate x of a Brownian particle in a periodic or constant potential is expected to show

* It should be noted that rigid walls are unsuitable as boundary conditions, because they would stop the current for any value of the applied field.

diffusive behaviour for $t \to \infty$. This can be seen by writing eq. (6.1.10) in the form

$$\langle u(t')\, u(t'')\rangle = kT\chi_u(|t'-t''|) \tag{6.1.21}$$

and integrating over t' and t'' between 0 and t, which yields

$$\langle [x(t)-x(0)]^2\rangle = 2kT \cdot t \int_0^t (1-\tau/t)\,\chi_u(\tau)\,\mathrm{d}\tau\,. \tag{6.1.22}$$

It can be shown that $\int_0^\infty \tau\chi_u(\tau)\,\mathrm{d}\tau = \mathrm{d}\chi_u(\omega)/\mathrm{d}(\mathrm{i}\omega)|_{\omega=0} < \infty$. Therefore, one obtains asymptotically for $t \to \infty$

$$\langle [x(t)-x(0)]^2\rangle \sim 2\,kT\chi_u^{(s)} \cdot t \equiv 2\bar{D}_x t\,, \tag{6.1.23}$$

where $\bar{D}_x$ is a renormalized position-diffusion constant related to the static mobility $\chi_u^{(s)}$ by an Einstein relation

$$\bar{D}_x = kT\chi_u^{(s)}\,. \tag{6.1.24}$$

In the Smoluchowski limit one finds [5, 148]

$$\begin{aligned}\bar{D}_x &= D_x\left\{\frac{1}{L}\int_0^L \exp[U(x)/kT]\,\mathrm{d}x \cdot \frac{1}{L}\int_0^L \exp[-U(x)/kT]\,\mathrm{d}x\right\}^{-1} \\ &\leq D_x\,,\end{aligned} \tag{6.1.25}$$

where L is the period.

For a sine-potential, the mobility χ_u is studied numerically in ref. [131].

For a constant potential, one finds the well-known result for free Brownian motion

$$\left.\begin{aligned}\chi_u(\omega) &= \frac{1}{m(\gamma-\mathrm{i}\omega)} \\ \chi_x(\omega) &= \frac{1}{-\mathrm{i}\omega m(\gamma-\mathrm{i}\omega)}\end{aligned}\right\} \text{ for all } \omega\,, \tag{6.1.26}$$

which agrees with the $\omega_0 \to 0$ limit of the harmonic oscillator. The position-diffusion constant takes the value

$$D_x = kT/m\gamma = D_u/\gamma^2\,. \tag{6.1.27}$$

in agreement with the Smoluchowski result (6.1.8).

6.2. Nonlinear conductance

We consider a simple electric circuit consisting of a nonlinear resistance element R, e.g. a p–n diode, in contact with a heat bath at temperature T, and driven by a current source I^{ext} (fig. 7). The element has a capacity represented by the constant capacitance C, such that the voltage V across the element is related to the charge Q by $V = Q/C$. The nonlinearity is described by a voltage-dependent conductance $G(Q) > 0$, which will in general depend parametrically on temperature. On the deterministic level, the relaxation towards the steady state Q_s $G(Q_s) = C I^{\text{ext}}$ is governed by the phenomenological law

$$\dot{Q} = -G(Q)\, Q/C + I^{\text{ext}}. \tag{6.2.1}$$

We use this system to discuss in some detail the problems which arise in constructing a stochastic model in such a nonlinear situation. We disregard the discrete nature of the charge and treat Q as a continuous stochastic variable. The current fluctuations induced by the coupling to the heat bath are modelled by Gaussian white noise modulated by a state-dependent amplitude $b(Q)$ (multiplicative noise). We thus write the nonlinear Ito–SDE (see section 2.4)

$$\mathrm{d}Q = v(Q)\,\mathrm{d}t + b(Q) \bullet \mathrm{d}w(t), \tag{6.2.2}$$

and the corresponding Fokker–Planck equation

$$\frac{\partial p(Q,t)}{\partial t} = -\frac{\partial}{\partial Q}[v(Q)\, p(Q,t)] + \frac{\partial^2}{\partial Q^2}[D(Q)\, p(Q,t)] \tag{6.2.3}$$

where the drift $v(Q)$ and the diffusion coefficient $D(Q) = \frac{1}{2}[b(Q)]^2$ are two as yet undetermined functions of Q.

In the driven case $I^{\text{ext}} \neq 0$, little can be said about the stochastic process on the basis of the phenomenological law (6.2.1) alone, even if we regard I^{ext} as a nonfluctuating quantity. The only general condition which the stochastic process must satisfy is that it is macroscopically compatible with (6.2.1) (see below). It is true that the probability current vanishes in the stationary state, i.e. the "potential condition" (4.4.17) is satisfied, and the stationary distribution $P_s(Q)$ is given explicitly by eq. (4.4.18),

$$p_s(Q) = Z^{-1} \exp[-\Phi(Q)] \tag{6.2.4}$$

with a distribution potential $\Phi(Q)$ obtained by integration of (4.4.19),

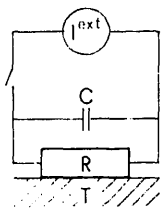

Fig. 7. Nonlinear resistance element R with intrinsic capacitance C driven by external current I^{ext}, and in contact with heat bath at temperature T.

$$\frac{\mathrm{d}\Phi}{\mathrm{d}Q} = -\frac{1}{D(Q)}\left[v(Q) - \frac{\mathrm{d}D(Q)}{\mathrm{d}Q}\right]. \tag{6.2.5}$$

However, this just determines $p_s(Q)$ for given functions $v(Q)$ and $D(Q)$, but in the driven case does not represent any condition on these functions.

In the case of the open circuit $I^{\mathrm{ext}} = 0$, on the other hand, the steady state is a thermodynamic equilibrium state, in which case we have the additional information that the stationary distribution has the canonical form

$$p_s(Q) = Z^{-1} \exp(-Q^2/2CkT), \tag{6.2.6}$$

since $E = Q^2/2C$ is the energy of the charged capacitance. This yields a relation between $v(Q)$ and $D(Q)$ of the form

$$v(Q) = -\frac{Q\,D(Q)}{CkT} + \frac{\mathrm{d}D(Q)}{\mathrm{d}Q}. \tag{6.2.7}$$

Together with the condition of macroscopic compatibility, this relation essentially determines the process, except for finite-size corrections, as we will now show.

If $G = G_0$ were independent of Q (linear conductance), we could set $v(Q) = -G_0 Q/C$, and obtain from (6.2.7) for the constant diffusion coefficient D_0 the Einstein relation

$$D_0 = kT\,G_0. \tag{6.2.8}$$

For the nonlinear conductance $G(Q)$ we introduce the hypothesis of a generalized Einstein relation as put forward in refs. [132a, b]

$$D(Q) = kT\,G(Q). \tag{6.2.9}$$

With this ansatz, we obtain from (6.2.7) for the Ito–Drift

$$v(Q) = -G(Q)\,Q/C + kT\,\mathrm{d}G(Q)/\mathrm{d}Q, \tag{6.2.10}$$

i.e. a correction to the deterministic law (6.2.1). It should be noted that the fluctuation-induced drift (2.4.12)

$$v^{\mathrm{f}}(Q) = \tfrac{1}{2} b\,\mathrm{d}b/\mathrm{d}Q = \tfrac{1}{2} kT\,\mathrm{d}G(Q)/\mathrm{d}Q \tag{6.2.11}$$

amounts to only half the correction in (6.2.10), such that the Stratonovich drift

$$u(Q) = v(Q) - v^{\mathrm{f}}(Q) = -G(Q)\,Q/C + \tfrac{1}{2} kT\,\mathrm{d}G(Q)/\mathrm{d}Q \tag{6.2.12}$$

also deviates from the deterministic law.

In the Fokker–Planck equation, the extra term may be combined with the diffusion term such that

$$\frac{\partial p(Q,t)}{\partial t} = \frac{\partial}{\partial Q}\left[G(Q)\frac{Q}{C}p(Q,t) + kT\,G(Q)\frac{\partial p(Q,t)}{\partial Q}\right], \tag{6.2.13}$$

which corresponds to a different separation of the probability current into drift and diffusion (see refs. [133, 134]),

$$\begin{aligned} j(Q,t) &= v(Q)\,p(Q,t) - \frac{\partial}{\partial Q}[D(Q)\,p(Q,t)] \\ &= -G(Q)\frac{Q}{C}p(Q,t) - kT\,G(Q)\frac{\partial p(Q,t)}{\partial Q}. \end{aligned} \tag{6.2.14}$$

In order to discuss the significance of these deviations of the drift from the deterministic law (6.2.1), we recall that the latter has to be understood as the asymptotic law for large systems ("thermodynamic limit"), and study the dependence of the various terms on a size parameter Ω, e.g. the cross-sectional area of the p–n junction. We introduce the intensive variable $q = Q/\Omega$ and denote Ω-independent quantities by a bar, such that $C = \bar{C}\Omega$, $G(Q) = \bar{G}(q)\,\Omega$. The important fact to realise is that the current fluctuations scale with $\Omega^{1/2}$, i.e.

$$b(Q) = \bar{b}(q)\,\Omega^{1/2} \tag{6.2.15}$$

whence

$$D(Q) = \bar{D}(q)\,\Omega, \tag{6.2.16}$$

and drift and diffusion coefficient in the Fokker–Planck equation for $p(q,t)$ become $-q\,\bar{G}(q)/\bar{C} + (kT/\Omega)\,\mathrm{d}\bar{G}(q)/\mathrm{d}q$ and $\bar{D}(q)/\Omega$, respectively. The ansatz (6.2.9) is consistent with the scaling (6.2.16) and eqs. (6.2.10) and (6.2.12) show that the deviations of the drift from the deterministic law (6.2.1) are of order Ω^0, i.e. represent finite-size corrections:

$$v(Q) = -\Omega q\,\bar{G}(q)/\bar{C} + \mathrm{O}(\Omega^0). \tag{6.2.17}$$

This result shows that in thermodynamic equilibrium the nonlinear Einstein relation (6.2.9) guarantees the compatibility of the stochastic description with the deterministic law in the thermodynamic limit.* Deviations from the ansatz (6.2.9) may, in fact, occur, but at most of order Ω^0, in order not to violate this compatibility. Such deviations amount to higher-order terms in the fluctuations (6.2.15).

We have thus obtained some understanding of the remarkable fact that phenomenological laws like (6.2.1) hold in the thermodynamic limit independent of the stochastic preparation of the system. It is important to realize that this is true only for the leading term in Ω. For size effects in the conductance, i.e. deviations of $G(Q)$ from $\Omega\,\bar{G}(q)$, the phenomenological law is expected to depend on the stochastic preparation. Unfortunately, such effects are ordinarily too small for experimental investigation, except possibly at critical points where different Ω-scaling laws apply.

* Strictly speaking, the deterministic law (6.2.1) is a relation between mean values, whereas q and $G(q)$ in (6.2.17) are of course still fluctuating quantities. But the difference between $\{q\,\bar{G}(q)\}$ and $\langle\bar{G}(\langle q\rangle)\rangle$ will again scale with Ω^{-1}, i.e. represent another finite-size correction [135].

For small driving currents, one may perform a perturbation expansion around the thermodynamic equilibrium state. It is important to realize that the validity of this procedure is restricted to the terms linear in I^{ext}. In higher order, one has to take Joule heating and heat exchange with the reservoir into account, and the temperature of the sample (if it can still be defined) differs from the bath temperature. Thus, already the deterministic description (6.2.1) is incomplete, and has to be supplemented by a heat transport equation. Analogous complications arise in other driven systems.

We now calculate the linear response of the voltage $V = Q/C$ to the driving current I^{ext}, i.e. the *differential resistance* χ_V. The perturbed drift is

$$\hat{v}(Q, t) = v(Q) + I^{\text{ext}}(t), \tag{6.2.18}$$

yielding a gradient-type perturbation

$$\Gamma_1(t) = -I^{\text{ext}}(t)\, \partial/\partial Q \tag{6.2.19}$$

of the Fokker–Planck operator. Therefore, the linear response is given by eq. (5.2.4, 29). From the Gaussian character of the stationary distribution (6.2.6), we thus obtain the *Nyquist theorem*

$$\chi_V(\tau) = \frac{\theta(\tau)}{kT} \langle V(\tau)\, V(0) \rangle = \frac{\theta(\tau)}{kT} S_{VV}(\tau). \tag{6.2.20}$$

Because the Fokker–Planck operator defined by (6.2.3) satisfies the condition of strict detailed balance (4.4.19) with $\sigma = \bar{\sigma}$, $\theta Q = Q$, it has only real eigenvalues. Therefore, $\chi_V(\tau)$ is a monotonically decreasing function,

$$1/C = \chi_V(\tau = 0) \geq \chi_V(\tau) > 0. \tag{6.2.21}$$

In the case of a linear conductance $G = G_0$, the Fokker–Planck operator has eigenvalues $\lambda_n = -nG_0/C$ (see section 3.2.E2), but $\chi_V^0(\tau)$ consists only of a single relaxation term,

$$\chi_V^0(\tau) = \frac{1}{C} \theta(\tau) \exp(-G_0 \tau / C) \tag{6.2.22}$$

i.e.

$$\chi_V^0(\omega) = \frac{1}{G_0 - \mathrm{i}\omega C} \tag{6.2.23}$$

in agreement with the deterministic result.

For small nonlinearity,

$$G(Q) = G_0(1 + \alpha Q + \beta Q^2), \tag{6.2.24}$$

one may perform a perturbation expansion in α and β [136, 137]. One finds that to first order in α and β, $\chi_V(\tau)$ still is a single exponential with an eigenvalue shifted linearly with β (clearly, the eigenvalues

can depend only on even powers of α). The higher eigenvalues enter with amplitudes starting with second order in α and β.

6.3. Bistable tunnel diode

Of specific interest are driven nonlinear systems in which the nonlinearity leads to instabilities and bistable behaviour in certain ranges of the driving forces. Following Landauer [82] we consider here a tunnel diode with a current-voltage characteristic shown in fig. 8, driven by a current source. Disregarding fluctuations, the system has for currents $I < I_l$ one stable stationary state with voltage $V_{s1}(I)$, for currents I such that $I_l < I < I_u$ two stable stationary states with $V_{s1}(I)$ and $V_{s2}(I)$ and an unstable one with $V_{s3}(I)$, and for $I > I_u$ again one stable stationary state with $V_{s2}(I)$. For $I \nearrow I_u$ and $I \searrow I_l$, the states $V_{s1}(I)$ and $V_{s2}(I)$, respectively, loose their stability, and a switching occurs to the other stable state. The tunnel diode thus represents a driven system showing a discontinuous (1st order-type) non-equilibrium phase transition between a low-voltage state V_{s1} and a high voltage state V_{s2}.

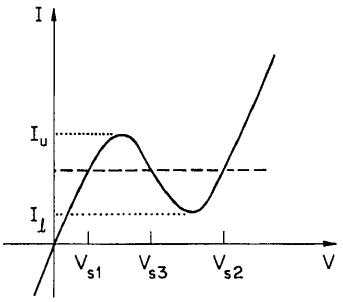

Fig. 8. Static current-voltage characteristic $I(V)$ of a tunnel diode. For currents I between I_l and I_u there exist two stable stationary states V_{s1} and V_{s2} and one unstable stationary state V_{s3}.

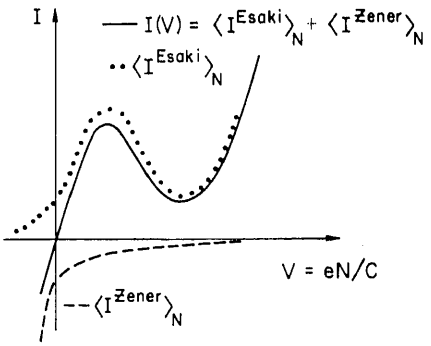

Fig. 9. Esaki current (· · ·) and Zener current (– – –) contributing to the static characteristic.

In a stochastic description, this phenomenon of bistability generates a number of interesting problems. In particular, there arises the question of how to reconcile the deterministic bistability with the existence of a unique stationary probability distribution. For the study of these problems, one needs a stochastic model valid under arbitrary driving conditions. As discussed in the preceding subsection, little can be said about such a model on general grounds. Therefore, we construct a stochastic model based on specific knowledge of the underlying physical processes for this particular system. We still disregard, however, the complications due to Joule heating and heat transfer to the environment which in principle always occur in driven systems. Essentially the same model describes a variety of other discontinuous transitions, e.g. chemical instabilities [9, 84, 86, 138, 139], optical instabilities [140–143] and vapor condensation [83, 144–146].

We take the discrete nature of the charge into account, and describe the state of the system by the number N of unit charges on the diode capacitance C. The voltage across the diode is then given by $V = eN/C$. The capacitance is charged by the sum of driving current I^{dr} and Zener current I^{Zener}, and discharged by the Esaki current I^{Esaki}. We assume that all contributions consist of uncorrelated transfers of single electrons. Then, they induce transitions between states N and $N \pm 1$ with transition rates

$$W(N+1,N) \equiv W^{+}(N) = [\langle I^{\mathrm{dr}}\rangle - \langle I^{\mathrm{Zener}}\rangle_N]/e \tag{6.3.1a}$$

$$W(N-1,N) \equiv W^{-}(N) = \langle I^{\mathrm{Esaki}}\rangle_N/e\,. \tag{6.3.1b}$$

One thus obtains a birth- and death-process described by the master equation

$$\frac{\mathrm{d}P(N,t)}{\mathrm{d}t} = W^{+}(N-1)\,P(N-1,t) + W^{-}(N+1)\,P(N+1,t) - [W^{+}(N)+W^{-}(N)]\,P(N,t)\,. \tag{6.3.2}$$

The dependence of the average currents $\langle I^{\mathrm{Esaki}}\rangle_N$ and $\langle I^{\mathrm{Zener}}\rangle_N$ on the voltage, i.e. on the state N of the system, may be taken from a microscopic model. The difference (see fig. 9)

$$I(V) = [\langle I^{\mathrm{Esaki}}\rangle + \langle I^{\mathrm{Zener}}\rangle]_{N=CV/e} \tag{6.3.3}$$

represents the static current–voltage characteristic of the diode. The current source is characterized by the average driving current $I^{\mathrm{ext}} = \langle I^{\mathrm{dr}}\rangle$, but fluctuations of I^{dr} (shot noise) are fully taken into account.

Since there cannot exist a stationary probability current along the N-axis, the stationary distribution P_{s} satisfies the condition (4.3.20) of strict detailed balance,

$$W^{-}(N+1)\,P_{\mathrm{s}}(N+1) = W^{+}(N)\,P_{\mathrm{s}}(N)\,, \tag{6.3.4}$$

from which one obtains immediately the solution

$$P_{\mathrm{s}}(N) = P_{\mathrm{s}}(N_0) \prod_{K=N_0}^{N-1} [W^{+}(K)/W^{-}(K+1)]\,. \tag{6.3.5}$$

This may be written in the form

$$P_{\mathrm{s}}(N) = Z^{-1} \exp[-\Phi(N)] \tag{6.3.6}$$

with the distribution potential

$$\Phi(N) = -\sum_{K=N_0}^{N-1} \ln[W^{+}(K)/W^{-}(K+1)]\,. \tag{6.3.7}$$

Maxima and minima of P_{s} occur at those values of N for which $W^{-}(N+1) = W^{+}(N)$, i.e. where

$$I^{\mathrm{ext}} = \langle I^{\mathrm{Esaki}}\rangle_{N+1} + \langle I^{\mathrm{Zener}}\rangle_N\,. \tag{6.3.8}$$

These are up to O(1) just the points on the bare characteristic (5.3.3) corresponding to $I = I^{\mathrm{ext}}$. Thus, in the bistable region, the probability distribution has two maxima at the deterministically stable states and a minimum at the unstable one.

For large systems one expects that the discrete nature of the charge becomes unimportant, and that a continuum description becomes possible. We therefore study the dependence on a size parameter Ω which we take again as the area of the diode junction. We introduce the intensive variable $n = N/\Omega$ with

the probability density $p(n) = \Omega P(N)$, and the transition rates per unit area

$$w^{\pm}(n) = W^{\pm}(\Omega n)/\Omega . \tag{6.3.9}$$

With this scaling, the Kramers–Moyal expansion (2.3.15) becomes an expansion in $1/\Omega$. Keeping terms up to $O(1/\Omega)$ we obtain the approximate Fokker–Planck equation

$$\frac{\partial p(n,t)}{\partial t} = -\frac{\partial}{\partial n}[v(n)\,p(n,t)] + \frac{\partial^2}{\partial n^2}[D(n)\,p(n,t)] \tag{6.3.10}$$

with the Ω-independent Ito-drift

$$v(n) = w^{+}(n) - w^{-}(n) \tag{6.3.11}$$

and the diffusion coefficient

$$D(n) = \frac{1}{2\Omega}[w^{+}(n) + w^{-}(n)] \equiv \frac{1}{\Omega}\bar{D}(n) \tag{6.3.12}$$

scaling as $1/\Omega$. The static characteristic (6.3.3) is determined by $v(n, I^{\mathrm{ext}}) = v(n,0) + (1/\Omega e)\, I^{\mathrm{ext}} = 0$, i.e.

$$I^{\mathrm{ext}} = I(V) \equiv -\Omega e v \;(n = \bar{C}V/e,\, I^{\mathrm{ext}} = 0), \tag{6.3.13}$$

where $\bar{C} = C/\Omega$ is the capacitance per unit area. From the detailed-balance condition, one obtains the stationary distribution (see eqs. (4.4.18a, b))

$$p_s(n) = Z^{-1} \exp[-\Phi^{\mathrm{FP}}(n)] \tag{6.3.14}$$

with the Fokker–Planck distribution potential

$$\Phi^{\mathrm{FP}}(n) = -\int_{n_0}^{n} \frac{1}{D(n')}\left[v(n') - \frac{\mathrm{d}D(n')}{\mathrm{d}n'}\right]\mathrm{d}n' . \tag{6.3.15}$$

The potentials (6.3.7) and (6.3.15) have leading terms of $O(\Omega)$, $\Phi(N) = \Omega\bar{\Phi}(n) + O(1)$, where

$$\bar{\Phi}(n) = -\int_{n_0}^{n} \ln\frac{w^{+}(n')}{w^{-}(n')}\,\mathrm{d}n' \tag{6.3.16}$$

$$\bar{\Phi}^{\mathrm{FP}}(n) = -2\int_{n_0}^{n} \frac{w^{+}(n') - w(n')}{w^{+}(n') + w^{-}(n')}\,\mathrm{d}n' \equiv -\int_{n_0}^{n} \frac{v(n')}{\bar{D}(n')}\,\mathrm{d}n' \tag{6.3.17}$$

respectively. This shows that the distributions (6.3.6), (6.3.14) become very strongly peaked at the deterministically stable states, with a width scaling as $\Omega^{-1/2}$.

The leading terms (6.3.16, 17) of the two potentials are not identical. Their derivatives differ by

$$\begin{aligned}\frac{\mathrm{d}\bar{\Phi}}{\mathrm{d}n}-\frac{\mathrm{d}\bar{\Phi}^{\mathrm{FP}}}{\mathrm{d}n} &= -\ln\frac{w^+(n)}{w^-(n)}+2\frac{w^+(n)-w^-(n)}{w^+(n)+w^-(n)} \\ &= -2\sum_{\nu=1}^{\infty}\frac{1}{2\nu+1}\left[\frac{w^+(n)-w^-(n)}{w^+(n)+w^-(n)}\right]^{2\nu+1},\end{aligned} \tag{6.3.18}$$

but the positions n_m of their minima and maxima defined by

$$w^+(n_m)=w^-(n_m)=w_m \tag{6.3.19}$$

coincide, and they have identical curvatures

$$\left.\frac{\mathrm{d}^2\bar{\Phi}}{\mathrm{d}n^2}\right|_{n_m}=\left.\frac{\mathrm{d}^2\bar{\Phi}^{\mathrm{FP}}}{\mathrm{d}n^2}\right|_{n_m}=-\frac{1}{w_m}\left.\frac{\mathrm{d}v(n)}{\mathrm{d}n}\right|_{n_m} \tag{6.3.20}$$

at these points. Therefore, in regions of width $\Omega^{-1/2}$ around the maxima and minima $n=n_m$, the two distributions are approximated by the same Gaussian or inverted Gaussian distributions, respectively (but possibly with different factors Z^{-1}). One has

$$p_{\mathrm{s}}(n)=Z^{-1}\exp\left\{-\frac{1}{2s_m}(n-n_m)^2\right\},\qquad n-n_m=\mathrm{O}(\Omega^{-1/2}), \tag{6.3.21}$$

where

$$s_m\equiv\frac{1}{\Omega}\bar{s}_m=\frac{1}{\Omega\bar{\Phi}''_m}=-\frac{\bar{D}_m}{\Omega}\left.\frac{1}{\mathrm{d}v/\mathrm{d}n}\right|_{n_m} \tag{6.3.22}$$

may be expressed in terms of the differential resistance ($R_m=(\mathrm{d}V/\mathrm{d}I)_m$) of the static characteristic (6.3.13). This yields

$$\bar{s}_m=\bar{D}_mR_mC=\bar{D}_n\bar{R}_m\bar{C}, \tag{6.3.23}$$

where $\bar{R}_m=\Omega R_m$ is the specific resistance of the junction in the state n_m.

On the other hand, a Fokker–Planck equation with Ito drift as in (6.3.11) and a diffusion coefficient

$$\tilde{D}(n)=\frac{1}{\Omega}\frac{w^+(n)-w^-(n)}{\ln w^+(n)-\ln w^-(n)}\qquad(>0) \tag{6.3.24}$$

has a stationary solution which agrees with the exact solutions in the leading terms of the exponents everywhere, and not only in the Gaussian regions around the maxima.

We have thus found that in the bistable region the stationary distribution consists of two peaks located at the deterministically stable states $V=V_1$, V_2, the larger peak representing the globally stable

state and the smaller one the metastable state. As I^{ext} increases from I_l to I_u, the height of the first peak decreases and the height of the second one increases, and at a critical current $I = I_c$ both peaks have the same height, i.e. the two states are equally probable. Because of the factor Ω in the exponent of $p_s(n)$, this transition occurs very abruptly in a current interval of O(1). The total weights p_1, p_2 of the two peaks are given by

$$\begin{aligned} p_2 = 1 - p_1 &= 1 - \exp[-\Omega(\bar{\Phi}_1 - \bar{\Phi}_2) + O(1)], \qquad \bar{\Phi}_1 > \bar{\Phi}_2 \\ &= \exp[-\Omega(\bar{\Phi}_2 - \bar{\Phi}_1) + O(1)], \qquad \bar{\Phi}_1 < \bar{\Phi}_2 , \end{aligned} \tag{6.3.25}$$

where $\bar{\Phi}_{1,2} = \bar{\Phi}(n_{1,2})$ are the minimum values of the potential $\bar{\Phi}(n)$. The current where $p_1 = p_2 = \frac{1}{2}$ coincides to O(1) with the critical current I_c where $\Phi_1 = \Phi_2$. For $I < I_c$, i.e. $\bar{\Phi}_1 < \bar{\Phi}_2$, practically all the weight is concentrated near state V_1, and for $I > I_c$, i.e. $\bar{\Phi}_1 < \bar{\Phi}_2$ near state V_2. The details of the transition in a current interval of O(1) depend on the terms of $O(\Omega)$ in the exponents. This behaviour shows that in the "thermodynamic limit" $\Omega \to \infty$, one obtains a first-order phase transition between a low-voltage phase $V_1(I)$ and a high-voltage phase $V_2(I)$ at the coexistence point $I = I_c$.

The dynamics of the system is determined by the spectrum of the master operator Γ. Since the process satisfies the condition of strict detailed balance (6.3.4, 4.3.20), Γ has only real eigenvalues. The behaviour of the low-lying eigenvalues may be discussed in a systematic way in the Fokker–Planck approximation. The Fokker–Planck operator may be symmetrized by the transformation (4.3.21), yielding the Schrödinger-like operator (4.4.20),

$$\Gamma^{symm} = \frac{d}{dn} D(n) \frac{d}{dn} - V(n), \tag{6.3.26}$$

with state-dependent mass $\hbar^2/2D(n) = \hbar^2\Omega/2\bar{D}(n)$ and effective potential (4.4.22)

$$\begin{aligned} V(n) &= \frac{1}{4} D(n) \left(\frac{d\Phi}{dn}\right)^2 - \frac{1}{2} \frac{d}{dn} \left(D(n) \frac{d\Phi}{dn}\right) \\ &= \frac{\Omega}{4} \bar{D}(n) \left(\frac{d\bar{\Phi}}{dn}\right)^2 - \frac{1}{2} \frac{d}{dn} \left(\bar{D}(n) \frac{d\bar{\Phi}}{dn}\right) + O(\Omega^{-1}), \end{aligned} \tag{6.3.27}$$

where we have dropped the superscript FP.

In the monostable regions $I < I_l$ and $I > I_u$, the first term has a single minimum of depth zero and curvature of $O(\Omega)$ at the state $n = n_m = n_1$ or n_2 corresponding to the stationary characteristic (6.3.13). The second term shifts the minimum down by an amount of O(1).

For the low-lying eigenvalues it is sufficient to use the Gaussian approximation (6.3.21) and a constant diffusion coefficient $\bar{D}_m = \bar{D}(n_m)$. With

$$\bar{\Phi}(n) = \frac{1}{2\bar{s}_m} (n - n_m)^2, \tag{6.3.28}$$

one obtains a harmonic-oscillator potential

$$V(n) = \frac{\Omega}{4} \frac{\bar{D}_m}{\bar{s}_m^2} (n - n_m)^2 - \frac{1}{2} \frac{\bar{D}_m}{\bar{s}_m} \tag{6.3.29}$$

giving rise to the spectrum

$$\lambda_{m,k} = k \cdot \lambda_m, \qquad \lambda_m = -\bar{D}_m/\bar{s}_m, \qquad k = 0, 1, 2, \ldots \tag{6.3.30}$$

Eq. (6.3.23) shows that $-\lambda_m$ is just the relaxation rate

$$-\lambda_m = 1/R_m C = 1/\bar{R}_m \bar{C} \tag{6.3.31}$$

of the equivalent RC-circuit. Anharmonic effects will play a role only for quantum numbers k of $O(\Omega)$.

For the spectral representation of the auto-covariance $S_{nn}(\tau) = \langle \Delta n(\tau)\, \Delta n(0) \rangle$ one needs the coefficients g_k and h_k defined in (3.2.14, 15). If these are expressed in terms of the harmonic-oscillator eigenfunctions $|k\rangle$, one finds

$$g_k = h_k = \langle k|n|0\rangle = \sqrt{\bar{s}_m/\Omega}\, \delta_{k,1}\,. \tag{6.3.32}$$

Thus, in the harmonic-oscillator approximation, only the first nonzero eigenvalue contributes to the charge fluctuations,

$$S_{nn}(\tau) = \frac{1}{\Omega}\, \bar{s}_m \exp(-|\lambda_m \tau|)\,. \tag{6.3.33}$$

With $V = en/\bar{C}$ one obtains the voltage auto-covariance S_{VV} by using (6.3.23) and (6.3.31)

$$S_{VV}(\tau) = \frac{e^2}{\Omega \bar{C}}\, \bar{D}_m\, \bar{R}_m \exp(-|\tau|/\bar{R}_m \bar{C}) \tag{6.3.34}$$

with the Fourier transform

$$S_{VV}(\omega) = \frac{e^2}{\Omega}\, \frac{2\bar{D}_m \bar{R}_m^2}{1 + (\omega \bar{R}_m \bar{C})^2}\,. \tag{6.3.35}$$

These relations have the form of a generalized Nyquist theorem.

Deviations from the harmonic-oscillator approximation give rise to higher "harmonics", i.e. terms with relaxation frequencies $k/\bar{R}_m \bar{C}$, $k > 1$.

In the bistable region $I_l < I < I_u$, one expects that the deterministic stability of the metastable state corresponds in the stochastic description to a very slow transition rate from the metastable to the globally stable state. In other words, one expects that for $\Omega \gg 1$ one eigenvalue of the stochastic operator becomes quasidegenerate with $\lambda_0 = 0$. This is indeed the case [42, 80–87]. Historically, this problem has been studied already by Kramers [42] in the context of the evaluation of a thermally activated escape rate. Extensions to a multi-dimensional situation have been discussed by Brinkman [80], Landauer and Swanson [81, 82] and Langer [83]. Recently, a detailed WKB-treatment has been given in ref. [87]. The problem has also been treated by an evaluation of the mean first-passage time [5, 147–150].

In this bistable region, the first term of the potential $V(n)$ in (6.3.27) has three minima of depth zero and curvature of $O(\Omega)$, two at the stable and metastable states n_1, n_2, and a third one at the unstable

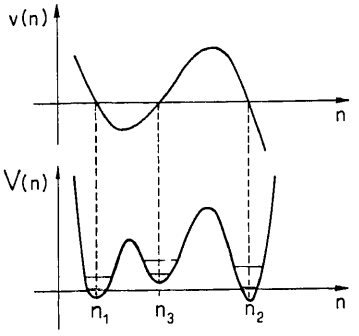

Fig. 10. Effective potential $V(n)$ of the Schrödinger-like master operator (6.3.26) of the tunnel diode in the bistable region.

state n_3. The second term shifts the minima at n_1 and n_2 downward and the minimum at n_3 upward by amounts of O(1) (see fig. 10).

Each of the low-lying eigenstates in this potential consists in good approximation of a harmonic-oscillator wave function in one of the three valleys. It can be characterized by two quantum numbers, $|m, k\rangle$, where $m = 1, 2, 3$ gives the number of the valley and $k = 0, 1, 2 \ldots$ describes the excitation level of the oscillator. Since valleys 1 and 2 are shifted downward and valley 3 is shifted upward, we find the eigenvalues

$$\left.\begin{aligned} \lambda_{1,k} &= k\lambda_1 \\ \lambda_{2,k} &= k\lambda_2 \\ \lambda_{3,k} &= (k+1)\lambda_3 \end{aligned}\right\}; \qquad \lambda_m = -\bar{D}_m/\bar{s}_m, \qquad k = 0, 1, 2, \ldots \tag{6.3.36a, b, c}$$

where in analogy to (6.3.22, 23)

$$\bar{s}_m = \frac{1}{|\bar{\Phi}''_m|} = \bar{D}_m |\bar{R}_m| \bar{C}, \tag{6.3.37}$$

such that

$$-\lambda_m = 1/|\bar{R}_m|\bar{C}. \tag{6.3.38}$$

Equations (6.3.36a, b) show that the two states $|1, 0\rangle$ and $|2, 0\rangle$ are degenerate. It is evident from fig. 10 that tunnelling between the two minima $m = 1, 2$ at the deterministically stable states will lift this degeneracy. One eigenvalue, λ_0, will remain zero, the other, λ_t, will assume an exponentially small negative value. It is this remaining quasi-degeneracy of the two lowest levels which corresponds to the deterministic stability of the metastable state. The correct linear combinations of the two harmonic-oscillator functions $|1, 0\rangle$ and $|2, 0\rangle$ corresponding to λ_0 and λ_t are found from normalization and orthogonality conditions as

$$|0\rangle = p_1^{1/2}|1, 0\rangle + p_2^{1/2}|2, 0\rangle \tag{6.3.39}$$

$$|t\rangle = p_2^{1/2}|1, 0\rangle - p_1^{1/2}|2, 0\rangle, \tag{6.3.40}$$

where $p_{1,2}$ are the weights given in (6.3.25). An evaluation of the tunnelling integral determining λ_t requires, however, an approximation in the overlap region near valley 3. An explicit calculation [84] yields for the left eigenfunctions φ_0, φ_t of the unsymmetrized operator Γ defined by (6.3.2)

$$\varphi_0 = 1 \tag{6.3.41}$$

$$\varphi_t = \frac{1}{2\sqrt{p_1 p_2}}\left\{p_2 - p_1 - \operatorname{erf}\sqrt{\frac{\Omega}{2|\bar{s}_3|}}(n - n_3)\right\} \tag{6.3.42}$$

with eigenvalues

$$\lambda_0 = 0$$

$$\lambda_t = -\frac{1}{2}\frac{1}{\sqrt{2\pi\Omega|\bar{s}_3|}}\frac{2w(n_3)\,p_s(n_3)}{p_1 p_2} \tag{6.3.43}$$

$$\sim -\exp\{-\Omega\,[\bar{\Phi}(n_3) - \bar{\Phi}_{ms}]\} \tag{6.3.44}$$

where $\operatorname{erf} x = 2\pi^{-1/2}\int_0^x \exp(-y^2)\,dy$ is the error function, and $\bar{\Phi}_{ms}$ is the metastable minimum of the potential $\bar{\Phi}(n)$ given by $\bar{\Phi}(n_2)$ or $\bar{\Phi}(n_1)$, depending on whether $I < I_c$ or $I > I_c$, respectively.

The sequence of the higher eigenvalues depends on the relative magnitude of the values of $\bar{R}_m$ of the three states. In the next approximation, each eigenfunction is changed by small admixtures of harmonic-oscillator functions in the other valleys of such signs, that it exhibits the proper number of nodes.

Interestingly, the eigenstate $|3, 0\rangle$ corresponding to the deterministically unstable state n_3 has an eigenvalue $\lambda_{3,0} = \lambda_3 = O(1)$, i.e. of the same order as the excited states in the other valleys. Thus, of the three zero-eigenvalues of the backward operator of the deterministic motion, only the two which correspond to the deterministically stable states n_1, n_2 change continuously, whereas the third one corresponding to n_3 changes discontinuously with the onset of fluctuations.

For the coefficients g_k and h_k determining the auto-covariance $S_{nn}(\tau)$ one finds in the bistable region, neglecting exponentially small overlap terms

$$g_t = h_t = \langle t|n|0\rangle = \sqrt{p_1 p_2}\,(n_1 - n_2) \tag{6.3.45a}$$

$$g_{m,k} = k_{m,k} = \langle m, k|n|0\rangle = \sqrt{\frac{p_m \bar{s}_m}{\Omega}}\,\delta_{k,1} \qquad (m = 1, 2) \tag{6.3.45b}$$

$$g_{3,k} = h_{3,k} = 0\,, \tag{6.3.45c}$$

yielding the voltage auto-covariance

$$S_{VV}(\tau) = p_1 p_2\,(V_1 - V_2)^2 \exp(-|\lambda_t \tau|)$$

$$+\frac{e^2}{\Omega\bar{C}}\{p_1\bar{D}_1\bar{R}_1 \exp(-|\tau|/\bar{R}_1\bar{C}) + p_2\bar{D}_2\bar{R}_2 \exp(-|\tau|/\bar{R}_2\bar{C})\}. \tag{6.3.46}$$

The first term which represents the contribution of the slow mode λ_t is exponentially small because of the prefactor $p_1 p_2$, and of the two remaining terms which are of the form (6.3.34) there survives only the one corresponding to the absolutely stable state, except in the immediate neighbourhood of the

transition point $I = I_c$ where the two weights p_1, p_2 are of comparable magnitude. Thus, also in the bistable region, the voltage auto-covariance $S_{VV}(\tau)$ is still given by (6.3.34, 35) with values $\bar{D}_m$ and $\bar{R}_m$ corresponding to the absolutely stable state. Only in a region of width $1/\Omega$ around the transition point, there occur anomalous voltage fluctuations of O(1) (instead of $O(\Omega^{-1/2})$) of extremely low frequency $\omega \sim |\lambda_t|$, corresponding to slow transitions between the two stable states.

Anomalous (nonstationary) fluctuations of a similar nature play an important role in the decay of a distribution concentrated near the unstable state n_3 ($I_l < I < I_u$). The representation by a Gauss process with positive $\dot{\rho}_0$ (see remark after (2.2.46)) is then a good approximation only in the initial time region of the relaxation process. For the intermediate time region, one needs a nonlinear theory of relaxation of the type discussed in refs. [151–155].

It should be noted that realistic diodes are well in the asymptotic limit of large Ω: In dimensionless units, the size parameter Ω is represented by the number N of carriers on the junction at some standard voltage, which is of order 10^8 for a junction of area $10^{-5}\,\mathrm{cm}^2$, capacitance $C \sim 10^{-11}\mathrm{F}$, at a voltage of 0.5 V. The relaxation time $1/|\lambda_t|$ is therefore astronomically large.

We finally discuss the linear response of the diode to a change of the average driving current,

$$\hat{I}^{\mathrm{ext}}(t) \equiv \langle I^{\mathrm{dr}}(t)\rangle = I^{\mathrm{ext}} + \delta I^{\mathrm{ext}}(t)\,. \tag{6.3.47}$$

This perturbation is represented by a state-independent modulation $\delta W(t) = \delta I^{\mathrm{ext}}(t)/e$ of the transition rate $W^+(N)$ (see (6.3.1a)), yielding a perturbation $\Gamma'(t) = \hat{\Omega}\,\delta W(t)$ of the master operator with the matrix*

$$\hat{\Omega}(N, M) = \delta_{N,M+1} - \delta_{N,M}\,. \tag{6.3.48}$$

The response variable defined by (5.2.1) may be expressed in terms of the distribution potential Φ as

$$\vartheta(N) = \exp[\Phi(N) - \Phi(N-1)] - 1\,, \tag{6.3.49}$$

or, using (6.3.7), in explicit form

$$\vartheta(N) = [W^-(N) - W^+(N-1)]/W^+(N-1)\,. \tag{6.3.50}$$

In the Fokker–Planck approximation, the perturbation is represented by the differential operator

$$\hat{\Omega} = -\frac{1}{\Omega}\frac{\partial}{\partial n} + \frac{1}{2\Omega^2}\frac{\partial^2}{\partial n^2} \tag{6.3.51}$$

which yields

$$\vartheta^{\mathrm{FP}}(n) = \frac{1}{\Omega}\frac{\mathrm{d}\Phi^{\mathrm{FP}}}{\mathrm{d}n} + \frac{1}{2\Omega^2}\left[\left(\frac{\mathrm{d}\Phi^{\mathrm{FP}}}{\mathrm{d}n}\right)^2 - \frac{\mathrm{d}^2\Phi^{\mathrm{FP}}}{\mathrm{d}n^2}\right] \tag{6.3.52a}$$

$$= \mathrm{d}\bar{\Phi}^{\mathrm{FP}}/\mathrm{d}n + \tfrac{1}{2}(\mathrm{d}\bar{\Phi}^{\mathrm{FP}}/\mathrm{d}n)^2 + \mathrm{O}(\Omega^{-1}) \tag{6.3.52b}$$

$$= -v/\bar{D} + \tfrac{1}{2}(v/\bar{D})^2 + \mathrm{O}(\Omega^{-1})\,. \tag{6.3.52c}$$

* In this section, we denote the operator defined in (5.1.2) by $\hat{\Omega}$, in order to distinguish it from the size parameter Ω.

The two expressions (6.3.49, 50) and (6.3.52) differ even in their leading terms, except in regions of width $\Omega^{1/2}$ around the stationary points where the two potentials (6.3.16, 17) agree.

The function $\vartheta(n)$ determines the response $\chi(\tau)$ of the charge density n to $\delta W(t)$ by eq. (5.2.3). The spectral representation (5.2.13a) is determined by the coefficients $g_k^{(\varphi)}$ and $h_k^{(\vartheta)}$ defined in (5.2.15a,b). In the monostable regions, we may use the harmonic-oscillator approximation (6.3.28, 29). Then, $g_k^{(\varphi)}$ is given by (6.3.32), and

$$h_k^{(\vartheta)} = \langle k|\vartheta(n)|0\rangle . \tag{6.3.53}$$

The leading term in $1/\Omega$ of $\chi(\tau)$ is determined by the linear approximation to $\vartheta(n)$. One obtains from (6.3.52b) and (6.3.28)

$$\vartheta(n) = \frac{1}{\bar{s}_m}(n - n_m) + \mathrm{O}(n - n_m)^2 \tag{6.3.54}$$

yielding

$$h_k^{(\vartheta)} = \frac{1}{\bar{s}_m} g_1 \delta_{k,1} \tag{6.3.55}$$

and therefore

$$\begin{aligned} \chi(\tau) &= \frac{1}{\bar{s}_m} S_{nn}(\tau)\, \theta(\tau) \\ &= \frac{\theta(\tau)}{\Omega} \exp(-\tau/\bar{R}_m \bar{C}) . \end{aligned} \tag{6.3.56}$$

The resistance function $R(\tau)$ of the junction defined by

$$\delta V(t) = \int_0^\infty R(\tau)\, \delta I^{\mathrm{ext}}(t - \tau)\, \mathrm{d}\tau \tag{6.3.57}$$

which is related to $\chi(\tau)$ by

$$R(\tau) = \chi(\tau)/\bar{C}, \tag{6.3.58}$$

is thus given by

$$R(\tau) = \frac{\theta(\tau)}{C} \exp(-\tau/R_m C) . \tag{6.3.59}$$

Fourier transformation yields the frequency-dependent differential resistance

$$R(\omega) = \frac{R_m}{1 - \mathrm{i}\omega R_m C}, \tag{6.3.60}$$

which shows that the static differential resistance $R(\omega = 0)$ does in leading order in $1/\Omega$ in fact agree with the value $R_m = (\mathrm{d}V/\mathrm{d}I)_m$ obtained from the static characteristic (6.3.13).

Comparison of (6.3.59) with (6.3.34) shows that the resistance function is in leading order related to the voltage fluctuations by the fluctuation theorem

$$R(\tau) = \frac{1}{e^2 \bar{R}_m \bar{D}_m} S_{VV}(\tau)\, \theta(\tau)\,. \tag{6.3.61}$$

In the bistable region, $g_k^{(\varphi)}$ is given by (6.3.41a, b) and for $h_k^{(\vartheta)}$ one finds correspondingly

$$h_t^{(\vartheta)} = \langle t|\vartheta(n)|0\rangle = \sqrt{p_1 p_2}(\vartheta_1 - \vartheta_2) \tag{6.3.62a}$$

$$h_{m,k}^{(\vartheta)} = \frac{1}{\bar{s}_m} g_{m,1}\delta_{k,1} \qquad (m = 1, 2) \tag{6.3.62b}$$

$$h_{3,k}^{(\vartheta)} = 0\,, \tag{6.3.62c}$$

where $\vartheta_m = \vartheta(n_m)$. This yields

$$\chi(\tau) = \left\{ p_1 p_2 (n_1 - n_2)(\vartheta_1 - \vartheta_2) \exp(\lambda_t \tau) + \frac{1}{\Omega}\left[p_1 \exp(-\tau/\bar{R}_1\bar{C}) + p_2 \exp(-\tau/\bar{R}_2\bar{C})\right] \right\} \theta(\tau)\,. \tag{6.3.63}$$

Again, the first term and the term corresponding to the metastable state are exponentially small, except in the immediate neighbourhood of the transition point where the two weights p_1, p_2 are of comparable magnitude. Thus, also in the bistable region, the resistance is still given by (6.3.59, 60), and the fluctuation theorem (6.3.61) remains valid. Only in a region of width 1 around the transition point, there occurs at extremely low frequencies $\omega \sim 1/|\lambda_t|$ an anomalous contribution to the resistance,

$$\Delta R(\omega) = \frac{p_1 p_2}{\bar{C}} \frac{(n_1 - n_2)(\vartheta_1 - \vartheta_2)}{|\lambda_t| - \mathrm{i}\omega}\,, \tag{6.3.64}$$

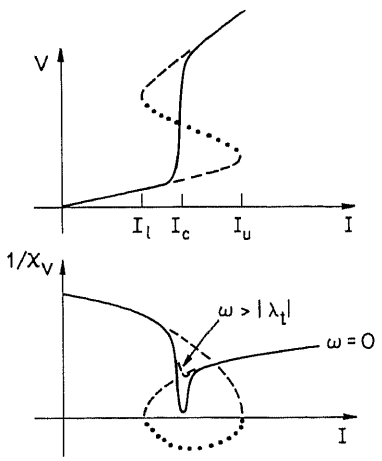

Fig. 11. Static voltage-current characteristic $V(I)$ and differential conductance $1/\chi_V$ of the tunnel diode. The stable and unstable parts of the deterministic characteristic and the deterministic differential conductance are represented by the dashed and dotted lines, respectively.

reflecting the asymptotically vertical (first-order) transition between the states n_1 and n_2. This behaviour is shown schematically in fig. 11.

6.4. Single-mode laser

Another driven nonlinear system showing an instability is the laser: At a critical pumping rate, the laser threshold, the state of incoherent radiation in the cavity becomes unstable against formation of a coherent state. This laser transition is continuous (2^{nd} order-type), in contrast to the discontinuous transition of the tunnel diode considered in the preceding subsection.

The laser has been treated in considerable detail at all levels of description [156–162]. Therefore, we restrict the discussion here to the simplest case of a single-mode laser (cavity in resonance with the atomic transition frequency ω_0), treated in rotating-wave approximation, in the limit that the electromagnetic loss rate is small compared to the atomic relaxation rates. Then, the atomic coordinates can be adiabatically eliminated, and the state of the laser is characterized by the complex-valued mode amplitude b which is normalized such that

$$N_{\mathrm{Ph}} = |b|^2; \qquad E = \hbar\omega_0 |b|^2 \tag{6.4.1}$$

are the total photon number and total electromagnetic energy in the cavity, respectively.

Near threshold, the deterministic behaviour is described by the equation

$$\dot{\boldsymbol{b}} = -\kappa \boldsymbol{b} + g^2(d - |b|^2)\boldsymbol{b} \tag{6.4.2}$$

for the two-component vector $\boldsymbol{b} = \{\mathrm{Re}b, \mathrm{Im}b\}$.

Here, the first term is the linear electromagnetic loss with loss rate κ, and the second term represents the nonlinear gain from the active medium, with d proportional to the pumping rate, and g^2 a normalized coupling constant. The laser threshold is determined by

$$g^2 d_c = \kappa\,, \tag{6.4.3}$$

and in terms of d_c, eq. (6.4.2) may be written

$$\dot{\boldsymbol{b}} = g^2[(d - d_c) - |b|^2]b\,. \tag{6.4.4}$$

This deterministic law would again be compatible with a large variety of stochastic models, as discussed in section 6.2. However, knowledge of the underlying physical processes allows the construction of a specific model. The mode-amplitude fluctuations are predominantly due to spontaneous emission noise, which near threshold may be modelled by additive complex-valued Wiener noise [156, 157]. One obtains a Fokker–Planck equation

$$\frac{\partial p(\boldsymbol{b}, t)}{\partial t} = -\frac{\partial}{\partial \boldsymbol{b}} \cdot [\boldsymbol{v}(\boldsymbol{b})\, p(\boldsymbol{b}, t)] + D \frac{\partial^2 p(\boldsymbol{b}, t)}{\partial \boldsymbol{b} \cdot \partial \boldsymbol{b}} \tag{6.4.5}$$

with drift

$$\boldsymbol{v}(\boldsymbol{b}) = g^2\,[(d - d_c) - b^2]\,\boldsymbol{b} \tag{6.4.6}$$

and a constant diffusion coefficient [156, 157]

$$D = \tfrac{1}{8}\kappa(1 + d_m/d_c)\,, \tag{6.4.7}$$

where d_m is the parameter value corresponding to complete inversion.

This process satisfies the condition of strict detailed balance (4.4.19) with $\bar{\sigma} = \sigma$, $\Theta \cdot \boldsymbol{b} = \boldsymbol{b}$, and vanishing odd drift vector, such that the distribution potential $\Phi(\boldsymbol{b})$ determining the stationary distribution

$$p_s(\boldsymbol{b}) = Z^{-1} \exp[-\Phi(\boldsymbol{b})] \tag{6.4.8}$$

is obtained as the solution of the differential equation (see (4.4.18a, b))

$$\frac{\partial \Phi}{\partial \boldsymbol{b}} = -\frac{1}{D}\boldsymbol{v}(\boldsymbol{b}) \tag{6.4.9}$$

in the form

$$\Phi(\boldsymbol{b}) = \frac{g^2}{2D}[-(d - d_c)b^2 + \tfrac{1}{2}b^4]\,. \tag{6.4.10}$$

Thus, below threshold ($d < d_c$), the distribution has a single peak at $b = 0$, whereas above threshold ($d > d_c$), there is a minimum at $b = 0$ and a maximum at a circular rim of radius $b = \sqrt{d - d_c}$ equal to the deterministic laser amplitude.

In order to study the size dependence, we introduce a size parameter Ω representing the length of the cavity. Eq. (6.4.1) shows that the mode amplitude scales as $b \propto \Omega^{1/2}$. Further, $g^2 \propto \Omega^{-1}$, $d \propto \Omega$, and $D \propto \Omega^0$, such that the probability distribution for the intensive variable $\bar{\boldsymbol{b}} = \boldsymbol{b}/\Omega^{1/2}$ satisfies again a Fokker–Planck equation with Ω-independent drift, and diffusion coefficient D/Ω, exactly as in the two preceding subsections. (Note that the diffusion coefficient D defined by (6.4.5) is Ω-independent.) Therefore, for large Ω the stationary distribution for $\bar{\boldsymbol{b}}$ becomes very narrow – at $d > d_c$ of course only in radial direction – with a width scaling as $\Omega^{-1/2}$.

It should be noted that a typical laser is thermodynamically a rather small system: In dimensionless units, the size parameter Ω is represented by the number N of photons at threshold, which is typically of the order 10^3. Thus, size effects are easier to observe in a laser than in other macroscopic systems [163, 164].

Because of strict detailed balance, the Fokker–Planck operator may be transformed by (4.3.21) into the Schrödinger-like operator

$$\Gamma^{\text{symm}} = D\frac{\partial}{\partial \boldsymbol{b}} \cdot \frac{\partial}{\partial \boldsymbol{b}} - V(b) \tag{6.4.11}$$

with constant mass $\hbar^2/2D$ and effective potential

$$V(\boldsymbol{b}) = \tfrac{1}{4}D(\partial\Phi/\partial \boldsymbol{b})^2 - \tfrac{1}{2}D\,\partial^2\Phi/\partial \boldsymbol{b} \cdot \partial \boldsymbol{b} \tag{6.4.12a}$$

$$= \frac{1}{4}\frac{g^4}{D}[(d - d_c)^2 - b^2]^2 b^2 + g^2[(d - d_c) - 2b^2]\,. \tag{6.4.12b}$$

Below threshold, $d < d_c$, $V(\boldsymbol{b})$ has a single minimum at $\boldsymbol{b} = 0$. For $d_c - d = O(\Omega)$, the low-lying eigenstates of energy and width of O(1) are well represented by the harmonic approximation

$$V(\boldsymbol{b}) = \frac{1}{4}\frac{g^4}{D}(d_c - d)^2 b^2 - g^2 (d_c - d) . \tag{6.4.13}$$

Anharmonic effects will play a role only for excitations of energy of $O(\Omega)$ and width of $O(\Omega^{1/2})$. The Schrödinger equation of the two-dimensional harmonic oscillator may be separated in polar coordinates, giving rise to the azimuthal and radial quantum numbers m and k, respectively. The eigenvalues are given by

$$\lambda_{m,k} = (|m| + 2k)\lambda_1, \qquad \begin{matrix} m = 0, \pm 1, \pm 2, \ldots \\ k = 0, 1, 2, \ldots \end{matrix} \tag{6.4.14}$$

where

$$\lambda_1 = -g^2 |d_c - d| . \tag{6.4.15}$$

The zero-point energy has been compensated by the last term of (6.4.13), thus guaranteeing $\lambda_{0,0} = 0$. All relaxation rates show a critical slowing down for $d \nearrow d_c$. The value of $|\lambda_1|$ agrees with the deterministic relaxation frequency following from (6.4.4).

Above threshold, $d > d_c$, $V(\boldsymbol{b})$ exhibits two types of minima, one on the circle $b_0 = \sqrt{d - d_c}$ corresponding to the deterministically stable state, the other at $b = 0$ corresponding to the unstable state (fig. 12). For $d - d_c = O(\Omega)$, the low-lying eigenstates (except for degeneracies, see below) are concentrated near one of the minima, and are well represented by the approximations

$$V(\boldsymbol{b}) = \frac{g^4}{D}(d - d_c)^2 (b - b_0)^2 - g^2 (d - d_c) \tag{6.4.16}$$

near $b = b_0$, where $b = \sqrt{b_1^2 + b_2^2}$ is the radial component, and

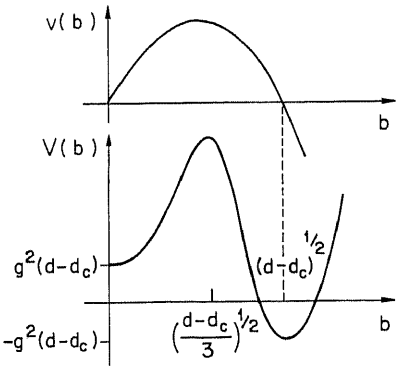

Fig. 12. Effective potential $V(b)$ of the Schrödinger-like master operator (6.4.12a, b) of the single-mode laser above threshold.

$$V(b) = \frac{1}{4}\frac{g^4}{D}(d-d_c)^2 b^2 + g^2(d-d_c) \tag{6.4.17}$$

near $b = 0$. Then, each of the eigenstates can be characterized by the azimuthal and radial quantum numbers m and k, and a further index μ indicating whether the eigenfunction is concentrated near $b = b_0$ ($\mu = 1$) or near $b = 0$ ($\mu = 2$). Since the radius b_0 is of $O(\Omega^{1/2})$, the curvature of the circle can be neglected, and the eigenvalue problem for $\mu = 1$ separates into a one-dimensional harmonic-oscillator problem for the radial motion, and free propagation with wave-number $q = 2\pi m/2\pi b_0$ in azimuthal direction. One thus finds the eigenvalues

$$\lambda^{(1)}_{m,k} = k \cdot 2\lambda_1 - D\,m^2/b_0^2, \qquad m = 0, \pm 1, \pm 2, \ldots \quad k = 0, 1, 2 \ldots \tag{6.4.18b}$$

with λ_1 given by (6.4.15). For $\mu = 2$, one again has a two-dimensional harmonic oscillator with eigenvalues

$$\lambda^{(2)}_{m,k} = (|m| + 2k + 2)\lambda_1, \qquad m = 0, \pm 1, \pm 2, \ldots \quad k = 0, 1, 2, \ldots \tag{6.4.18b}$$

starting with $\lambda^{(2)}_{00} = 2\lambda_1$ because the potential (6.4.16) is shifted upward. The degeneracy between the states $|0, k+1, \mu = 1\rangle$ and $|0, k, \mu = 2\rangle$ is lifted by tunnelling between the two minima, leading to an exponentially small splitting.

The spectrum (6.4.18a) shows that the radial relaxation rates $|\lambda^{(1)}_{0,k}|$ harden again above threshold; the value of $|\lambda^{(1)}_{01}| = 2|\lambda_1|$ agrees with the radial relaxation frequency following from the deterministic equation (6.4.4). To the continuum of deterministically stable states $b = b_0$ with constant phase, on the other hand, there correspond in the stochastic description the slow phase-diffusion modes $\lambda^{(1)}_{m,0} = O(1/\Omega)$. Interestingly, the mode $|0, 0, \mu = 2\rangle$ corresponding to the deterministically unstable state $b = 0$ has a relaxation rate $|\lambda^{(2)}_{00}| = 2\lambda_1 = O(1)$, similar to the result for the tunnel diode.

In a critical region $d - d_c$ of O(1) around threshold, anharmonic effects become important. The spectrum has been studied in detail by Risken [156, 157]. The eigenvalues are of $O(\Omega^{-1/2})$ in this region and connect smoothly the asymptotic results (6.4.14) and (6.4.18a, b).

The amplitude auto-correlation matrix

$$\mathbf{S}(\tau) = \langle \boldsymbol{b}(t+\tau)\,\boldsymbol{b}(t)\rangle \tag{6.4.19}$$

is given by (3.2.14, 15) in terms of the coefficients $\boldsymbol{g}_k$, $\boldsymbol{h}_k$. Below threshold, one finds

$$\boldsymbol{g}_{m,k} = \boldsymbol{h}_{m,k} = \langle m, k|\boldsymbol{b}|0, 0\rangle = \sqrt{\frac{D}{2|\lambda_1|}}\,[\{1, -\mathrm{i}\}\delta_{m,1} + \{1, \mathrm{i}\}\delta_{m,-1}]\delta_{k,0}\,, \tag{6.4.20}$$

whence

$$\boldsymbol{g}_{1,0}\boldsymbol{h}^*_{1,0} + \boldsymbol{g}_{-1,0}\boldsymbol{h}^*_{-1,0} = \frac{D}{|\lambda_1|}\mathbf{1} \tag{6.4.21}$$

and therefore

$$\mathbf{S}(\tau) = \frac{D}{|\lambda_1|} \exp(-|\lambda_1 \tau|)\, \mathbf{1}, \qquad d < d_c\,, \tag{6.4.22}$$

with Fourier transform

$$\mathbf{S}(\omega) = \frac{2D}{\lambda_1^2 + \omega^2}\, \mathbf{1}, \qquad d < d_c\,. \tag{6.4.23}$$

Above threshold, one finds

$$\boldsymbol{g}^{(1)}_{m,k} = \boldsymbol{h}^{(1)}_{m,k} = \tfrac{1}{2} b_0 [\{1, -\mathrm{i}\}\delta_{m,1} + \{1, \mathrm{i}\}\delta_{m,-1}]\delta_{k,0}\,, \tag{6.4.24}$$

whereas the $\boldsymbol{g}^{(2)}_{m,k}$ are exponentially small. Therefore,

$$\mathbf{S}(\tau) = \tfrac{1}{2} b_0^2 \exp(-D|\tau|/b_0^2)\, \mathbf{1}, \qquad d > d_c\,, \tag{6.4.25}$$

with Fourier transform

$$\mathbf{S}(\omega) = \frac{D}{(D/b_0)^2 + \omega^2}\, \mathbf{1}, \qquad d > d_c\,. \tag{6.4.26}$$

In the critical region $d - d_c = \mathrm{O}(1)$ around threshold, higher modes will contribute to the amplitude fluctuations because of anharmonicity. Their effect is, however, very small, and amounts only to about 2% [156, 157].

We finally discuss the linear response of the laser to an external coherent field at the laser frequency, modulated with a time-dependent amplitude $\boldsymbol{b}^{\mathrm{ext}}(t)$, which is injected into the cavity. The nonlinear gain of the laser depends on the total field $\boldsymbol{b}^{\mathrm{tot}} = \boldsymbol{b} + \boldsymbol{b}^{\mathrm{ext}}$ whereas the electromagnetic loss is independent of $\boldsymbol{b}^{\mathrm{ext}}$. Therefore, the effect of the external field is taken into account by replacing the deterministic equation (6.4.2) by

$$\dot{\boldsymbol{b}} = -\kappa \boldsymbol{b} + g^2 (d - |\boldsymbol{b} + \boldsymbol{b}^{\mathrm{ext}}|^2)(\boldsymbol{b} + \boldsymbol{b}^{\mathrm{ext}})\,. \tag{6.4.27}$$

Linearizing in $\boldsymbol{b}^{\mathrm{ext}}$ and neglecting terms in the perturbation which vanish at threshold yields

$$\dot{\boldsymbol{b}} = g^2 (d - d_c - |\boldsymbol{b}|^2)\, \boldsymbol{b} + \kappa\, \boldsymbol{b}^{\mathrm{ext}}(t)\,. \tag{6.4.28}$$

Thus, near threshold the external field gives rise to a state-independent extra drift,

$$\hat{\boldsymbol{v}}(\boldsymbol{b}, t) = \boldsymbol{v}(\boldsymbol{b}) + \kappa\, \boldsymbol{b}^{\mathrm{ext}}(t)\,, \tag{6.4.29}$$

and the operator $\hat{\boldsymbol{\Omega}}$ describing the perturbation $\Gamma'(t) = \hat{\boldsymbol{\Omega}} \cdot \boldsymbol{b}^{\mathrm{ext}}(t)$ of the master operator is given by

$$\hat{\boldsymbol{\Omega}} = -\kappa\, \partial/\partial \boldsymbol{b}\,. \tag{6.4.30}$$

Since this is of the gradient form (5.2.28), the susceptibility tensor describing the response of the laser field $\boldsymbol{b}$ to the external field $\boldsymbol{b}^{\text{ext}}$ is given by the fluctuation theorem (5.2.33),

$$\chi(\tau) = -\frac{\kappa}{D}\,\theta(\tau)\frac{\mathrm{d}}{\mathrm{d}\tau}\mathbf{S}(\tau)\,. \tag{6.4.31}$$

Below threshold, we thus find by using (6.4.22)

$$\chi(\tau) = \kappa\,\theta(\tau)\exp(-|\lambda_1|\tau)\,\mathbf{1}, \qquad d < d_c\,, \tag{6.4.32}$$

with Fourier transform

$$\chi(\omega) = \frac{\kappa}{|\lambda_1| - \mathrm{i}\omega}\,\mathbf{1}, \qquad d < d_c\,, \tag{6.4.33}$$

in agreement with the deterministic response following from (6.4.28).

Above threshold, (6.4.25) yields

$$\chi(\tau) = \tfrac{1}{2}\kappa\,\theta(\tau)\exp(-D\tau/b_0^2)\,\mathbf{1}, \qquad d > d_c\,, \tag{6.4.34}$$

with Fourier transform

$$\chi(\omega) = \frac{1}{2}\frac{\kappa}{(D/b_0^2) - \mathrm{i}\omega}\,\mathbf{1}, \qquad d > d_c\,, \tag{6.4.35}$$

whereas the deterministic response following from (6.4.28) is anisotropic, depending on whether $\boldsymbol{b}^{\text{ext}}$ is parallel ($\parallel$) or perpendicular ($\perp$) to the spontaneous laser amplitude $\boldsymbol{b}$:

$$\chi_{\parallel}^{\text{det}}(\omega) = \frac{\kappa}{2g^2(d - d_c) - \mathrm{i}\omega} \tag{6.4.36a}$$

$$\chi_{\perp}^{\text{det}}(\omega) = \frac{\kappa}{-\mathrm{i}\omega}\,. \tag{6.4.36b}$$

6.5. Stochastic Ising model

We consider a system of N Ising spins* $x_l(t) = \pm 1$, $l = 1, \ldots, N$, which interact with each other and with a heat bath at temperature T. The interaction with the bath induces transitions between spin configurations $\boldsymbol{x} = \{x_1, \ldots, x_N\}$. We restrict the discussion to single-spin-flip models, i.e. we assume random jumps between configurations $\boldsymbol{x}$ which differ by the reversal of a single spin only, such that the total spin is not conserved.

Such a process may serve as a model for a variety of physical systems. Some applications are listed in table 6.1.

* We use the rather unconventional notation x_l for the spin variables, in accordance with the notation used for the two-state process.

Table 6.1

System	Variables	Bath	System – bath interaction
Uniaxial magnet	Spins $x_l = \pm 1$ at lattice sites l	Phonons	Spin–phonon interaction
Crystal with off-center atoms (e.g. hydrogen-bonded ferro-electrics)	Positions $Q_l = \pm Q$ of atom in lattice cell l	Phonons	Pseudospin–phonon interaction
Molecular crystal with 2 molecular orientations (e.g. NH_4Cl)	Orientation of molecule l	Phonons	Pseudospin–phonon interaction
Physisorbed layer	Occupation number $n_l = 0, 1$ of lattice site l	Vapor	Sorption–Desorption
Helix-coil system	State of bond of base pair l (intact or broken)	Solvent	Oxidation–reduction

On the other hand, the single-spin-flip model cannot describe systems in which the total spin $X = \Sigma_l x_l$ is conserved, such as binary mixtures with constant concentrations etc.

We denote by $S_l^- \boldsymbol{x}$ the configuration with spin x_l reversed. The time evolution of a single-spin-flip process is then described by a master equation of the form [19, 165]

$$\frac{\partial p(\boldsymbol{x}, t)}{\partial t} = \sum_l [W(\boldsymbol{x}, S_l^- \boldsymbol{x})\, p(S_l^- \boldsymbol{x}, t) - W(S_l^- \boldsymbol{x}, \boldsymbol{x})\, p(\boldsymbol{x}, t)] . \tag{6.5.1}$$

In the stationary state, the system is in thermal equilibrium. Therefore, the stationary distribution has the canonical form

$$p_s(\boldsymbol{x}) = Z^{-1} \exp[-E(\boldsymbol{x})/kT] , \tag{6.5.2}$$

where $E(\boldsymbol{x})$ is the energy of the configuration $\boldsymbol{x}$. Further, the process satisfies the condition of detailed balance (4.3.17), where $\tilde{\sigma}$ is the time-reversed process. Since for Ising dynamics one has $\Gamma_{\tilde{\sigma}}(\bar{\boldsymbol{y}}, \bar{\boldsymbol{x}}) = \Gamma_{\sigma}(\boldsymbol{y}, \boldsymbol{x})$, independent of the time-reversal behaviour of the x_l (true spins or pseudo-spins), the transition rates satisfy the condition (4.3.20) of strict detailed balance

$$W(\boldsymbol{x}, \boldsymbol{y})\, p_s(\boldsymbol{y}) = W(\boldsymbol{y}, \boldsymbol{x})\, p_s(\boldsymbol{x}) . \tag{6.5.3}$$

For single-spin-flip process, it follows that the expression

$$\begin{aligned} &W(\boldsymbol{x}, S_l^- \boldsymbol{x}) \exp\{[E(\boldsymbol{x}) - E(S_l^- \boldsymbol{x})]/kT\} \\ &\quad = W(S_l^- \boldsymbol{x}, \boldsymbol{x}) \exp\{[E(S_l^- \boldsymbol{x}) - E(\boldsymbol{x})]/kT\} \equiv \bar{W}_l(\boldsymbol{x}^{(l)}) \end{aligned} \tag{6.5.4}$$

is independent of spin x_l, i.e. depends only on the configuration $\boldsymbol{x}^{(l)}$ of the set of all spin except spin x_l. The energy difference

$$E(S_l^- \boldsymbol{x}) - E(\boldsymbol{x}) = 2 F_l^{\mathrm{mol}}(\boldsymbol{x}^{(l)})\, x_l \tag{6.5.5}$$

defines the molecular field $F_l^{\mathrm{mol}}(\boldsymbol{x}^{(l)})$ acting on spin x_l. In terms of this molecular field, the transition rate takes the form

$$\begin{aligned} W(\boldsymbol{x}, S_l^- \boldsymbol{x}) &= \bar{W}_l(\boldsymbol{x}^{(l)}) \exp[x_l F_l^{\mathrm{mol}}(\boldsymbol{x}^{(l)})/kT] \\ &= \tfrac{1}{2} A_l(\boldsymbol{x}^{(l)}) \{1 + x_l \tanh[F_l^{\mathrm{mol}}(\boldsymbol{x}^{(l)})/kT]\}, \end{aligned} \tag{6.5.6}$$

where the $A_l(\boldsymbol{x}^{(l)})$ are unspecified functions of the configurations $\boldsymbol{x}^{(l)}$. For translationally invariant systems, $A_l(\boldsymbol{x}^{(l)}) = A(\boldsymbol{x}^{(l)})$.

Because of the strict detailed-balance symmetry (6.5.3) all eigenvalues of the master operator are real (and nonpositive), i.e. the processes described by the stochastic Ising model are relaxation processes. An oscillatory process cannot be described by such a model.

If $E(\boldsymbol{x})$ is a sum of two-spin interactions and single-spin (Zeeman) terms,

$$E(\boldsymbol{x}) = -\frac{1}{2} {\sum_{ll'}}' J_{ll'} x_l x_{l'} - \sum_l F_l x_l \tag{6.5.7}$$

then

$$F_l^{\mathrm{mol}}(\boldsymbol{x}^{(l)}) = \sum_{l'} J_{ll'} x_{l'} + F_l . \tag{6.5.8}$$

In the Glauber model [19, 165], one takes $A_l(\boldsymbol{x}^{(l)}) = A(T)$ independent of $\boldsymbol{x}^{(l)}$ and assumes a linear chain with $F_l = 0$ and nearest-neighbour interactions $J_{ll'} = J(\delta_{l,l+1} + \delta_{l,l-1})$. Since for Ising variables

$$\tanh[C(x_{l+1} + x_{l-1})] = \tfrac{1}{2}(x_{l+1} + x_{l-1}) \tanh(2C), \tag{6.5.9}$$

one finds

$$W(\boldsymbol{x}, S_l^- \boldsymbol{x}) = \tfrac{1}{2} A(T) [1 + \tfrac{1}{2} B(T)\, x_l (x_{l+1} + x_{l-1})] \tag{6.5.10}$$

with $B(T) = \tanh(2J/kT)$.

For this model, the complete spectrum of the stochastic operator is available [19, 165]. It is easy to determine the lowest branches by using the left eigenfunctions φ_n (see subsection 3.2). One finds

$$\varphi^{(0)}(\boldsymbol{x}) = 1 , \qquad \lambda^{(0)} = 0 , \tag{6.5.11}$$

corresponding to the stationary state;

$$\varphi_q(\boldsymbol{x}) = N^{-1/2} \sum_l x_l \exp(\mathrm{i}ql), \qquad \lambda_q = -A(T)[1 - B(T)\cos q] \tag{6.5.12}$$

corresponding to the relaxation of spin-density waves of wave number q with relaxation frequencies $|\lambda_q|$; and

$$\varphi_{Q,q}(x) = N^{-1} \sum_{ll'} (x_l x_{l'} - \langle x_l x_{l'} \rangle) \sin(q|l-l'|) \exp\left[\frac{\mathrm{i}}{2} Q(l+l')\right] \tag{6.5.13}$$

$$\lambda_{Q,q} = -2A(T)\left[1 - B(T)\cos\frac{Q}{2}\cos q\right],$$

where $\langle x_l x_{l'} \rangle = [\tanh(J/kT)]^{|l-l'|}$, related to the decay of quadratic functions of the spin variables. Eigenfunctions of higher than second degree in the spin variables may be found by using special spin functions introduced in ref. [166], or the stochastic operator may be diagonalised by a transformation to fermion operators [167].

We now consider the linear response to forces $F_l(t)$ coupling to the Ising spins x_l with an interaction energy

$$E_1(x) = -\sum_l x_l \, \delta F_l(t) . \tag{6.5.14}$$

We assume that the only effect of the forces $\delta F_l(t)$ is to modulate the transition rates by the time-dependent molecular field

$$\hat{F}_l(x^{(l)}, t) = F_l(x^{(l)}) + \delta F_l(t) . \tag{6.5.15}$$

Then, the perturbed process has the accompanying distribution

$$p_a(x, \delta F) \propto p_s(x) \exp\left(\sum_l x_l \delta F_l / kT\right) . \tag{6.5.16}$$

From eqs. (5.2.23, 25), we find

$$\psi_l(x) = \xi_l / kT; \qquad \xi = x - \langle x \rangle , \tag{6.5.17}$$

which yields for the susceptibility matrix $\chi_{ll'}(\tau)$ the fluctuation theorem (5.2.26),

$$\chi_{ll'}(\tau) = -\frac{\theta(\tau)}{kT}\frac{\partial}{\partial\tau}\langle \xi_l(\tau)\, \xi_{l'}(0)\rangle \tag{6.5.18}$$

$$= -\frac{\theta(\tau)}{kT}\frac{\partial S_{ll'}(\tau)}{\partial\tau}$$

with the spatial Fourier transform

$$\chi_q(\tau) = -\frac{\theta(\tau)}{kT}\frac{\partial S_q(\tau)}{\partial\tau} . \tag{6.5.19}$$

For the Glauber model (6.5.9), the spatial Fourier transforms x_q of the spin variables x_l are just the left eigenfunctions $\varphi_q(x)$ given in (6.5.12), and bacause of the detailed balance symmetry the right eigenfunctions are $\psi_q(x) = \varphi_q(x)\, p_s(x)/\langle|\varphi_q|^2\rangle$. Therefore, the spectral representation (5.2.13b) of the

susceptibility χ_q is

$$\chi_q(\tau) = -\theta(\tau)\,\lambda_q g_q h_{-q}\,\exp(\lambda_q \tau) \tag{6.5.20}$$

with

$$g_q = \frac{1}{kT}\frac{\langle x_q \varphi_{-q}\rangle}{\langle|\varphi_q|^2\rangle} = \frac{1}{kT} \tag{6.5.21}$$

$$h_q = \langle x_{-q}\varphi_q\rangle = \langle|\varphi_q|^2\rangle = (\lambda_0/\lambda_q)\exp(2J/kT).$$

Therefore, one obtains

$$\chi_q(\tau) = \frac{\theta(\tau)}{kT}|\lambda_0|\,\exp\left(\frac{2J}{kT}\right)\exp(\lambda_q\tau) \tag{6.5.22}$$

or in the frequency domain

$$\chi_q(\omega) = \frac{1}{kT}\exp\left(\frac{2J}{kT}\right)\frac{\lambda_0}{\lambda_q + \mathrm{i}\omega}, \tag{6.5.23}$$

with the eigenvalues λ_q given in (6.5.12).

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Note added in proof:

The following books and review articles deal with the same subject area and provide additional insight.

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