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Stochastic processes I: Asymptotic behaviour and symmetries[1])

by **P. Hänggi**[2])

Institut für Physik, Universität Basel, Switzerland

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Abstract. Various features of Markov processes describing statistical systems in equilibrium and nonequilibrium are discussed. We study the spectral properties of stochastic operators and the consequences for the asymptotic behaviour of solutions of general master equations. In this context we introduce the concept of ergodic classes in state space and extremal probabilities. Furthermore, we investigate the symmetry properties of stochastic processes. We discuss the consequences for stochastic processes of both: symmetry transformations in state space and symmetry properties obtained by interchanging the time arguments in the joint-probability (generalized detailed balance). Various symmetry relations for multivariate probabilities and multi-time correlation functions are obtained. In addition, a necessary and sufficient operator condition for the generalized detailed balance symmetry is derived.

1. Introduction

Our concern here will be to present a phenomenological theory of macroscopic systems which are not necessarily in a thermodynamic equilibrium. For the description of systems in terms of a finite set of degrees of freedom which do not behave in a deterministic way but display statistical fluctuations of the system variables, the theory of stochastic processes plays an important role. Statistical fluctuations always reflect a lack of knowledge about the exact state of the total system, either because of quantum noise, or because of the impossibility of keeping track of the huge number of uncontrolled fine-grained variables. They may also be imposed on the system from the outside by random external forces, e.g. by coupling the system to reservoirs. The interactions between all the degrees of freedom may lead to a cooperative behaviour of the system. Such cooperative systems can then usually be described in terms of a small number of collective state variables (macrovariables) obtained through a coarse-graining in phase space. The theory of continuous time-parameter stochastic processes has been applied with good success to the description of such cooperative phenomena in nonequilibrium systems [1–5]. Particularly, a treatment with in general multidimensional Markov processes turns out to be successful.

The following work on real stochastic Markov processes is organized as follows: In the first part we derive some useful stochastic equations for Markov processes, needed for the description of the fluctuation dynamics in physical systems, and discuss

[1]) Work supported by Swiss National Science Foundation.

[2]) Present address: Department of Physics, University of Illinois, Urbana, Illinois 61801 USA.

the main properties of those equations. Loosely spoken the Markov principle states that the future of the dynamics depends only on the present dynamics. We present the description of continuous Markov processes in terms of stochastic differential equations. By introducing a generalization of the Stratonovitch stochastic integral we clear up some differences in recent physical works on continuous Markov processes. In Section 3 we investigate the spectral properties of the stochastic operators and the consequences for the asymptotic behaviour of solutions of the stochastic equations. In this context we introduce the concept of ergodic classes in state space and extremal probabilities. In Section 4 we study the symmetry properties of stochastic processes. We discuss the consequences of both: symmetry transformations in state space and symmetry properties obtained by interchanging the time arguments in the joint-probability of stationary Markov processes (generalized detailed balance). Various symmetry relations for multivariate probabilities and multi-time correlation functions are given; in addition a necessary and sufficient operator condition for generalized detailed balance is derived.

2. Stochastic equations for Markov processes

The different dynamical behaviour of a set of macrovariables $\mathbf{x} = (x_1, \ldots, x_n)$ forming the state space Σ can be treated in a unified way in terms of master equations. The stochastic properties of the system are then characterized by probability functions $p(\mathbf{x}t)$ defined in the state space Σ. Next we study the differential equations governing the time evolution of, in general, real time-inhomogeneous strong Markov processes $\mathbf{x}(t)$ [5–9].[3] In the following we use the notation: $\mathbf{x}(t)$ for the stochastic process itself, and $\mathbf{x}(t)$, for the random variables at time t or a single value in the configuration space Σ. The specific interpretation of $\mathbf{x}(t)$ will be understood from the context. Using usual operator notation, the semi-group property of the conditional probability $R(\mathbf{x}t \mid \mathbf{y}t_1)$, $t \geq t_1$, reads [5–9] (Chapman–Kolmogorov equation)

$$R(t \mid t_1) = R(t \mid s)R(s \mid t_1), \quad t \geq s \geq t_1 \tag{2.1}$$

with

$$R(t^+ \mid t) = \mathbb{1}. \tag{2.2}$$

Note that the conditional probability where $s < t_1$, $R(\mathbf{y}s \mid \mathbf{x}t_1) = R(\mathbf{x}t_1 \mid \mathbf{y}s) \times p(\mathbf{y}s)/p(\mathbf{x}t_1)$, will depend on $p(\mathbf{x}t_1)$ so that

$$R(t \mid t_1)p(t_1) = R(t \mid s)R(s \mid t_1)p(t_1), \quad s < t_1 < t, \quad \forall p(t_1), \tag{2.3a}$$

but

$$R(t \mid t_1) \neq R(t \mid s)R(s \mid t_1), \quad s < t_1 < t. \tag{2.3b}$$

Hence, the time ordering in the *linear* transition function operator $R(t \mid t_1)$, $t \geq t_1$, which coincides with the linear conditional probability $R(t \mid t_1)$, $t \geq t_1$, plays an important role. The semigroup R can be generated from the infinitesimal propagator

$$R(t + dt \mid t) = \mathbb{1} + \Gamma(t)\, dt, \quad dt > 0, \tag{2.4a}$$

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[3]) We always deal with non-terminating processes, where the parameter t is not a random variable but varies in $t \in [t_0, +\infty)$.

where (see also equation (2.7a))

$$\Gamma(t) = \frac{d}{dr} R(r \mid t)\bigg|_{r=t^+} = -\frac{d}{dt} R(r \mid t)\bigg|_{r=t^+} \tag{2.4b}$$

is the generator of the semi-group acting on a Banach space Π of ~~bounded functions~~ measures [8–9]. A process for which the derivatives of $R(t \mid s)$ with respect to the times t and s exist will be called stochastically differentiable. From the semi-group property we obtain the 'forward equation' [5–9]

$$\frac{dR(t \mid s)}{dt} = \Gamma(t)R(t \mid s), \quad t \geq s, \tag{2.5}$$

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

$$R(t \mid s) = R(t \mid s + ds)R(s + ds \mid s), \quad ds > 0, \tag{2.6}$$

the 'backward equation' [5–9]

$$\frac{dR(t \mid s)}{ds} = -R(t \mid s)\Gamma(s), \quad t \geq s, \tag{2.7a}$$

involving differentiation with respect to the *former* time s. In terms of the transpose operator R^+

$$R^+(\mathbf{x}t \mid \mathbf{y}s) = R(\mathbf{y}t \mid \mathbf{x}s), \tag{2.8}$$

the backward equation reads

$$\frac{dR^+(t \mid s)}{ds} = -\Gamma^+(s)R^+(t \mid s), \quad t \geq s. \tag{2.7b}$$

The formal solution of the forward and backward equation can be written

$$R(t \mid t_1) = \mathscr{T} \exp \int_{t_1}^{t} \Gamma(s)\, ds, \quad t \geq t_1, \tag{2.9}$$

where $\mathscr{T}$ is the time-ordering operator. From a physical point of view, the interest in the forward and backward equation lies in the fact that they yield equations of motions for the single-event probabilities and for conditional expectations. Applying both sides of equation (2.5) to $p(s)$ we obtain the 'master equation'

$$\frac{dp(t)}{dt} = \Gamma(t)p(t). \tag{2.10}$$

This equation shows that the in general non-symmetric generator $\Gamma(t)$ determines the dynamics of a Markov process in the same sense as the Hamiltonian determines the dynamics of a (Markovian) Hamiltonian system. With the solution of equation (2.10) and the Markov property for the conditional probabilities

$$R(\mathbf{x}_n t_n | \mathbf{x}_{n-1} t_{n-1}, \ldots, \mathbf{x}_1 t_1) = R(\mathbf{x}_n t_n \mid \mathbf{x}_{n-1} t_{n-1}), \tag{2.11a}$$

where

$$t_n \geq t_{n-1} \geq \cdots \geq t_1, \tag{2.12}$$

we have for the multivariate probability $p^{(n)}(\mathbf{x}_1 t_1, \ldots, \mathbf{x}_n t_n)$ the useful result

$$p^{(n)}(\mathbf{x}_1 t_1, \ldots, \mathbf{x}_n t_n) = \prod_{i=2}^{n} R(\mathbf{x}_i t_i \mid \mathbf{x}_{i-1} t_{i-1}) p(\mathbf{x}_1 t_1). \tag{2.13}$$

Moreover, equation (2.13) yields the 'inverse' Markovian property

$$R(\mathbf{x}_1 t_1 \mid \mathbf{x}_2 t_2, \ldots, \mathbf{x}_n t_n) = R(\mathbf{x}_1 t_1 \mid \mathbf{x}_2 t_2). \tag{2.11b}$$

The conditional expectation $\langle f(t) \mid \mathbf{y}(s) \rangle$ of a bounded state function $f(\mathbf{x}, t)$ is defined as the mean taken over the subset of sample functions passing through state $\mathbf{y}$ at time s.

$$\langle f(t) \mid \mathbf{y}(s) \rangle = \int f(\mathbf{x}t) R(\mathbf{x}t \mid \mathbf{y}s)\, d\mathbf{x}, \tag{2.14}$$

or using operator notation

$$\langle f(t) \mid s \rangle = R^{+}(t \mid s) f(t), \quad t \geq s. \tag{2.15}$$

Hence, we obtain with equation (2.8)

$$\frac{d\langle f(t) \mid s \rangle}{ds} = -\Gamma^{+}(s) \langle f(t) \mid s \rangle, \quad t \geq s. \tag{2.16}$$

The conditional averages are therefore solutions of the backward equation. With respect to the time t, they satisfy the averaged forward equation augmented by a term resulting from the explicit time-dependence of $f(t)$

$$\frac{d}{dt} \langle f(t) \mid s \rangle = \langle \Gamma^{+}(t) f(t) \mid s \rangle + \left\langle \frac{\partial f(t)}{\partial t} \middle| s \right\rangle, \quad t \geq s. \tag{2.17}$$

All the equations (2.10–2.17) are important in the derivation of master equations in the theory of stochastic differential equations.

The properties of the in general non-symmetric operator $\Gamma(t)$ defined on space Π ~~of bounded measurable functions~~ are different depending on whether the sample functions are continuous (continuous processes) or discontinuous. For discontinuous Markov processes it is convenient to represent the stochastic kernel $\Gamma(\mathbf{x}, \mathbf{y}; t)$ in terms of two other functions

$$\Gamma(\mathbf{x}, \mathbf{y}; t) = W(\mathbf{x}, \mathbf{y}; t) - \delta(\mathbf{x} - \mathbf{y}) V(\mathbf{y}, t), \tag{2.18}$$

where

$$V(\mathbf{y}, t) = \int W(\mathbf{x}, \mathbf{y}; t)\, d\mathbf{x} \geq 0, \tag{2.19}$$

yielding the stochastic property (preservation of normalization of probabilities)

$$\int \Gamma(\mathbf{x}, \mathbf{y}; t)\, d\mathbf{x} = 0. \tag{2.20}$$

The function $W(\mathbf{x}, \mathbf{y}; t)$ is the transition probability per unit time in which the process takes on a value in $(\mathbf{x}, \mathbf{x} + d\mathbf{x})$ when it starts at state $\mathbf{y}$. $V(\mathbf{y}, t)$ is the transition probability per unit time in which the process takes on a value different from $\mathbf{y}$ when it starts at the value $\mathbf{y}$. The mathematical conditions that there exists a *unique* solution for an *honest* conditional probability

$$\int R(\mathbf{x}t \mid \mathbf{y}s)\, d\mathbf{x} = 1, \quad \text{for all } t, s; t > s, \tag{2.21}$$

which satisfies both the forward and backward equation, are discussed for time-homogeneous processes elsewhere [10] (conservative stochastic processes). Using equation (2.18) the master equation can be written in its usual form [1, 5]

$$\frac{\partial p(\mathbf{x}t)}{\partial t} = \int \{W(\mathbf{x}, \mathbf{y}; t)p(\mathbf{y}t) - W(\mathbf{y}, \mathbf{x}; t)p(\mathbf{x}t)\}\, d\mathbf{y}. \tag{2.22}$$

Using the Kramers–Moyal expansion [11–12], where

$$\begin{aligned}\Gamma(\mathbf{x}, \mathbf{y}; t) &= \int \Gamma(\mathbf{z}, \mathbf{y}; t)\, \delta(\mathbf{z} - \mathbf{x})\, d\mathbf{z} \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \delta^{(n)}(\mathbf{y} - \mathbf{x}) \int (\mathbf{z} - \mathbf{y})^n \Gamma(\mathbf{z}, \mathbf{y}; t)\, d\mathbf{z} \qquad (2.23) \\ &= \sum_{n=1}^{\infty} \frac{1}{n!} A_n(\mathbf{y}, t)\, \delta^{(n)}(\mathbf{y} - \mathbf{x}); \qquad (2.24)\end{aligned}$$

the master equation can be converted into a differential operator of infinite order if all the moments A_n in equation (2.24) exist. As a consequence of the truncation Lemma by Pawula [13], a stochastic kernel $\Gamma(\mathbf{x}, \mathbf{y}; t)$, which consist's of a *finite* number of δ-functions and their derivatives contains *only* the distributions $\delta^{(1)}(\mathbf{x} - \mathbf{y})$ and $\delta^{(2)}(\mathbf{x} - \mathbf{y})$. The master equation obtained is of the following structure:

$$\frac{\partial p(\mathbf{x}t)}{\partial t} = -\nabla \cdot \mathbf{a}(\mathbf{x}, t)p(\mathbf{x}t) + \nabla\nabla : \mathbf{D}(\mathbf{x}, t)p(\mathbf{x}, t). \tag{2.25}$$

This master equation is the Fokker–Planck-equation with $\mathbf{a}(\mathbf{x}t)$ the drift vector and $\mathbf{D}(\mathbf{x}t)$ the diffusion matrix. A continuous Markov process, i.e. all the sample functions are almost all continuous functions, satisfies the Hincin conditions [8–9]: $\forall \epsilon > 0$

$$\int_{|\mathbf{x}-\mathbf{y}|>\varepsilon} R(\mathbf{x}t \mid \mathbf{y}s)\, d\mathbf{x} = o(t - s), \tag{2.26}$$

$$\int_{|\mathbf{x}-\mathbf{y}|\le\varepsilon} (\mathbf{x} - \mathbf{y})R(\mathbf{x}t \mid \mathbf{y}s)\, d\mathbf{x} = (t - s)\mathbf{a}(\mathbf{y}, s) + o(t - s), \tag{2.27}$$

$$\int_{|\mathbf{x}-\mathbf{y}|\le\varepsilon} (\mathbf{x} - \mathbf{y})^2 R(\mathbf{x}t \mid \mathbf{y}s)\, d\mathbf{x} = (t - s)\mathbf{b}(\mathbf{y}, s)\mathbf{b}^+(\mathbf{y}, s) + o(t - s), \tag{2.28}$$

such that

$$\mathbf{b}(\mathbf{x}t)\mathbf{b}^{+}(\mathbf{x}t) = 2\cdot\mathbf{D}(\mathbf{x}t).^{4}) \tag{2.29}$$

Here, $\mathbf{b}^{+}$ is the transposed matrix of $\mathbf{b}$. Using some mild mathematical properties on the coefficients in equations (2.27–2.29) [6, 8, 9], the master equation for these processes becomes the Fokker–Planck equation, equation (2.25). A continuous Markov process with the master equation of the form as equation (2.25) is equivalently described by the Ito stochastic differential equation [14–17]

$$d\mathbf{x}(t) = \mathbf{a}(\mathbf{x}(t), t)\,dt + \mathbf{b}(\mathbf{x}(t), t)\,d\mathbf{w}(t), \tag{2.30}$$

where $\mathbf{w}(t)$ is a vector of independent Wiener processes with

$$\langle w_i(t)\rangle = 0 \qquad \langle w_i^2(t)\rangle = t, \tag{2.31}$$

$$\langle w_i(t_2)w_i(t_1)\rangle = t_1 + (t_2 - t_1)\Theta(t_1 - t_2), \quad \forall i. \tag{2.32}$$

$\Theta(t_1 - t_2)$ denotes the step function.

Hence, we obtain the following description for continuous Markov processes: The condition in equation (2.26) amounts to the fact that in a small time interval the state of the process is almost sure to remain in the immediate neighbourhood of its initial state. The main part of a displacement is described by the regular drift $\mathbf{a}(\mathbf{x}t)$ in equation (2.27) and on this one superimposes the continuous random components characterizing the fluctuations with respect to the regular motion. By use of the definition of the Ito stochastic integral, equation (2.30) can be integrated to obtain the sample paths of the process

$$\mathbf{x}(t) = \mathbf{x}(t_o) + \int_{t_o}^{t} \mathbf{a}(\mathbf{x}(t), t)\,dt + \underset{\text{Ito}}{\int_{t_o}^{t}} \mathbf{b}(\mathbf{x}(s), s)\,d\mathbf{w}(s). \tag{2.33}$$

The Ito stochastic integral is defined by taking $\lambda = 1$ in the *generalized* Stratonovitch stochastic integral (GSI):

$$\underset{\text{GSI}}{\int_{t_o}^{t}} \mathbf{b}(\mathbf{x}(s), s)\,d\mathbf{w}(s) = \text{L.i.m.} \lim_{\Delta t\to 0^+} \sum_i \mathbf{b}\big(\lambda\mathbf{x}(t_i) + (1-\lambda)\mathbf{x}(t_i + \Delta t); t_i\big)[\mathbf{w}(t_i + \Delta t) - \mathbf{w}(t_i)]. \tag{2.34}$$

Historically Stratonovitch used $\lambda = \frac{1}{2}$ [18]. With a Taylor expansion about $\mathbf{x}(t_i)$ and the properties of the Wiener process in equations (2.31–2.32) the relationship

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[4]) An easily verified condition implying Hincin conditions is that of Kolmogorov: there exists a $\delta > 0$ such that

$$\int |\mathbf{x} - \mathbf{y}|^{2+\delta} R(\mathbf{x}t|\mathbf{y}s)\,d\mathbf{x} = o(t - s).$$

Indeed, for $k = 0, 1, 2$ we have

$$\int_{|\mathbf{x}-\mathbf{y}|>\varepsilon} |\mathbf{x} - \mathbf{y}|^{k} R(\mathbf{x}t\,|\,\mathbf{y}s)\,dx \le \frac{1}{\varepsilon^{2+\delta-k}} \int |\mathbf{x} - \mathbf{y}|^{2+\delta} R(\mathbf{x}t\,|\,\mathbf{y}s)\,d\mathbf{x} = o(t - s).$$

between the integrals can be calculated, yielding

$$\begin{aligned}\underset{\text{GSI}}{\int_{t_0}^{t}} \mathbf{b}(\mathbf{x}(s), s)\, d\mathbf{w}(s) &= \text{L.i.m.} \lim_{\Delta t \to 0^+} \sum_i \left\{ \mathbf{b}(x(t_i); t_i) + \left(\sum_n \sum_k \left(\frac{\partial b_{lj}}{\partial x_k} \right) b_{kn} \right.\right. \\ &\qquad \left.\left. \times [(\lambda - 1) w_n(t_i) + (1 - \lambda) w_n(t_i + \Delta t)] + \cdots \right)_{lj} \right\} \\ &\qquad \times [\mathbf{w}(t_i + \Delta t) - \mathbf{w}(t_i)] \\ &= \underset{\text{Ito}}{\int_{t_0}^{t}} \mathbf{b}(\mathbf{x}(s); s)\, d\mathbf{w}(s) + (1 - \lambda) \int_{t_0}^{t} \mathbf{F}(\mathbf{x}(s); s)\, ds, \end{aligned} \tag{2.35}$$

where

$$F_i(\mathbf{x}(s), s) = \sum_j \sum_k \frac{\partial b_{ij}(\mathbf{x}(s), s)}{\partial x_k} b_{kj}(\mathbf{x}(s), s). \tag{2.36}$$

Hence, the Ito stochastic differential equation, equation (2.30), with the correspondingly Fokker–Planck equation, equation (2.25), is equivalently described by the GSI stochastic differential equation:

$$d\mathbf{x}(t) = \mathbf{a}(\mathbf{x}(t), t)\, dt - (1 - \lambda)\mathbf{F}(\mathbf{x}(t), t)\, dt + \mathbf{b}(\mathbf{x}(t), t)\, d\mathbf{w}(t). \tag{2.37}$$

For $\lambda \neq 1$ and $\mathbf{x}$-dependent diffusion coefficients this description gives rise to a 'spurious' drift term corresponding to the noise coupled to the random functions b_{ij} on the right-hand side of equation (2.34). This fact clarifies the 'differences' in the formulation of stochastic properties in recent physical works with continuous Markov processes [1, 3, 19].

3. Spectral properties and asymptotic behaviour of probabilities

In the following we restrict the discussion, if not stated otherwise, to time-homogeneous Markov processes. All time-homogeneous Markov processes have the property that they do not improve the initial information. The time-independent generator Γ represents a *dissipative operator* [20], i.e. we have for the real part

$$\operatorname{Re}(f, \Gamma f) = \operatorname{Re} \int f^*(\mathbf{x}) \Gamma(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) p_{st}(\mathbf{x})\, d\mathbf{x}\, d\mathbf{y} \leq 0, \quad \forall f \in D(\Gamma). \tag{3.1}$$

According to the Phillips–Lumer theorem [20, 21], the stochastic generator Γ generates a *contraction semi-group* $R(\tau)$, $\tau \geq 0$ in Π:

$$\| R(\tau) f \| \leq \| f \|. \tag{3.2}$$

← total variation norm !

The spectrum $\{\lambda_\nu\}$ of the dissipative generator may consist in general of both a discrete and a continuous part with $\operatorname{Re} \lambda_\nu \leq 0$. For a time-homogeneous Markov process with a finite discrete state space, Γ is an ordinary stochastic matrix with the following interesting properties:

(1) All the eigenvalues of Γ are real or complex. Complex eigenvalues occur in pairs and the corresponding eigenvectors may be chosen complex conjugates of each other [6, 7, 22].[5])

(2) The sum of the elements of any eigenvector corresponding to a non-zero eigenvalues is zero, and the sum of the elements of an eigenvector with a zero eigenvalue may be chosen to be 1 [7, 22]. If Γ is double stochastic [7]

$$\sum_i \Gamma_{ij} = \sum_j \Gamma_{ij} = 0. \tag{3.3}$$

a stationary solution exists which is uniform: $p_{st}(i) = 1/N, \forall i.$

(3) For a v_o-fold latent root zero the rank of Γ is $N - v_o$, indicating the existence of v_o linear independent eigenvectors with eigenvalue zero [23]. N denotes the dimension of Γ or the number of states.

(4) For a birth and death process with N states and strictly positive transition rates all the eigenvalues are real and they are *not* degenerate [24]. Moreover, the eigenvalues of the stochastic matrix formed with the $N - 1$ residual states, $\Gamma^{(N-1)}$, separate those of $\Gamma = \Gamma^{(N)}$, i.e. [24]

$$0 = \lambda_o^{(N)} = \lambda_o^{(N-1)} > \lambda_1^{(N)} > \lambda_1^{(N-1)} > \cdots > \lambda_{N-1}^{(N)} > \lambda_{N-1}^{(N-1)} > \lambda_N^{(N)} \tag{3.3}$$

Further, a minimal region for the relaxation spectra in the complex plane can be constructed using for the matrix Γ little known general theorems; which are due to Gerschgorin [25, 26]:

(5) Every eigenvalue of the matrix Γ (Note that corresponding results may be obtained by working with the transpose, Γ^+, instead of Γ.) lies in at least one of the circular discs with centres Γ_{ii} and radii $r_i = \sum_{j \neq i} \Gamma_{ji}$. Notably, all the eigenvalues lie within the circle with centre at $\max_i \{\Gamma_{ii}\}$ and radius $R = \max_i \{-\Gamma_{ii}\}$. (See Fig. 1.) Hence we obtain explicitly:

(6) According to the preservation of normalization, equation (2.20), at least one eigenvalue is zero and the real part of a *non-zero* eigenvalue must be *negative definite*. So pure imaginary eigenvalues for Γ are impossible and the possibility of recurring probability solutions is therefore ruled out! Hence, the dynamics of a time-homogeneous system with a *finite* number of states can never be governed by a *unitary* one-parameter semi-group of transformations (Hamiltonian motion).

The second theorem of Gerschgorin yields even more detailed information concerning the distribution of the eigenvalues among the discs which can be constructed from Γ or its transpose Γ^+:

(7) If s of the circular discs of the theorem in (5) form a connected domain which is isolated from other discs, then there are precisely s eigenvalues of Γ within this connected domain.

(8) Detailed information about possible eigenvalues $\{\lambda_\nu\}$ of an irreducible stochastic matrix Γ which may lie on the border of maximum circle with radius R and centre $-R$ (see (5)) is obtained by studying the spectra of the non-negative matrix $\mathbf{A} = \Gamma + R\mathbb{1}$. Then, using the fact that $R^n = (\lambda + R)^n$ if $\mathbf{A}$ has n eigenvalues equal in modulus to R (Perron–Frobenius theorem [27]), the possible n eigenvalues on the border of the circle with radius R are

[5]) Note that the statement in [22]; that $|\mathrm{Re}\, \lambda_\nu| > |\mathrm{Im}\, \lambda_\nu|$ holds only for $N \leq 3$.

cyclic with values at

$$\lambda \in \left\{ -R + R \exp \frac{2\pi i k}{n}, \quad k = 0, 1, 2, \ldots, n - 1 \right\}.$$

This case occurs, e.g. in a cyclic system with constant transition rates, $\Gamma_{21} = \Gamma_{32} = \cdots = \Gamma_{1N} = \gamma > 0$; where:

$$\lambda_k = -\gamma + \gamma \exp\left(\frac{2\pi i k}{N}\right), \quad k = 0, \ldots, N-1. \tag{3.5}$$

The eigenvector components, $p_k(l)$, are given by:

$$p_k(l) = \frac{1}{N} \exp\left[(2\pi i k) l / N\right], \tag{3.6}$$

The results given here enable the study of the relaxation times in stochastic processes without solving the actual master equations. Particularly, one can estimate the long-time behaviour of certain correlation functions and the relaxation of mean values. As a simple example for these theorems, we give in Figure 1 the minimal region in the complex plane for the eigenvalues of the stochastic matrix Γ of the 3-state process

$$\Gamma = \begin{pmatrix} -2\frac{1}{2} & 0 & \frac{1}{2} \\ 2 & -3 & 0 \\ \frac{1}{2} & 3 & -\frac{1}{2} \end{pmatrix} \tag{3.7}$$

The eigenvalues of Γ are:

$$\lambda_o = 0, \qquad \lambda_{1/2} = -3 \pm i. \tag{3.8}$$

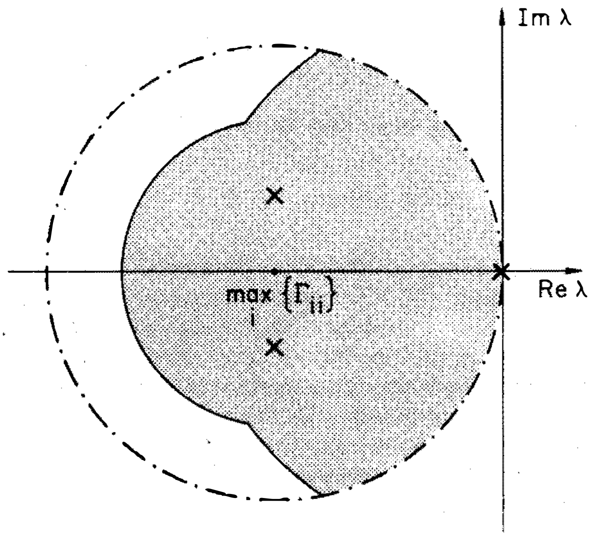

Figure 1
The shaded area gives the minimal region in the complex plane for the relaxation spectra of the 3-state process with generator Γ given in equation (3.7). The crosses denote the exact values for the relaxation constants and the dashed-dotted disc with radius $R = \max_i\{|\Gamma_{ii}|\}$ determines the region in the complex plane independent of any special form of the dissipative generator Γ.

The spectral properties of the stochastic generator Γ also influence the ergodic properties of the process. One usually deals with two kinds of ergodic theorems: there are those which are time versions of laws such as the law of large numbers [6, 8, 14, 28] and also those stating the existence of a limiting probability function independent of the way of preparation [19, 29]. As a consequence of the time evolution equation

$$p(t) = R(t)p(o), \tag{3.8}$$

all expectations and correlations will in general depend on the initial probability $p(o)$. It is of interest to know the conditions under which the statistical properties of the system become asymptotically independent of preparation effects. We shall call a process *ergodic*, if

$$\lim_{t \to +\infty} R(\mathbf{x}t \mid \mathbf{y}o) = p_{as}(\mathbf{x}), \quad \forall \mathbf{y} \in \Sigma \tag{3.9}$$

exists and $R(+\infty)$ represents a singular operator on Π mapping the probabilities $p(o)$ onto a unique asymptotic probability $p_{as} \in \Pi$ independent of $p(o)$. Note that we may have in general the following situations:

—an ergodic probability distribution which is unique.
—no limiting probability, i.e. the system disperses to infinity as time increases ($p_{as} \equiv 0$).
—several asymptotic probabilities whose number becomes infinite according to the *linearity* of the master equation.

The asymptotic properties of a discrete time-homogeneous Markov process with a finite number of states can be investigated as follows: the state space Σ can be portioned into classes $\{C\}$ by use of the equivalence relation $\sim$:

$$i \sim j: \quad \text{if } R(it \mid jo) \equiv R(i,j;t) > 0 \text{ and } R(j,i;t) > 0 \quad \text{for } \textit{some } t > 0. \tag{3.10}$$

The symmetry and reflexivity relation are trivial and the transitivity relation follows from the Kolmogorov equation

$$R(i, j, t + \tau) = \sum_k R(i, k; \tau)R(k, j; t) \quad \tau > 0, t > 0. \tag{3.11}$$

and the semi-positivity of the conditional probabilities. Equation (3.10) must hold only for some fixed time $t > 0$, because $R(i, j : t)$ is either identically zero or always positive in $(0, +\infty)$ [30]. We call a class C_i *ergodic*, C_i^{erg}, if in a given class every state is ergodic, i.e. $\lim_{t \to \infty} R(i, i; t) = p_i > 0$. This definition makes sense because in a given class C_i every state is ergodic or none are. We already know that there exists an infinite set of stationary asymptotic probabilities if more than one ergodic class exists. But we will show that this infinite number of different asymptotic probabilities can be characterized in terms of a linear combination of a finite number of special asymptotic probabilities $\{p_{st}^{\mu}\}$ (extremal probabilities)

$$\lim_{t \to +\infty} R(t)p(0) \equiv p_{as} = \sum_{\mu} \omega_{\mu} p_{st}^{\mu}. \tag{3.12}$$

The generator Γ can always be brought into a Jordan canonical form [27]

$$\mathbf{\Gamma} = \mathbf{H}^{-1}\mathbf{J}\mathbf{H}. \tag{3.13}$$

Because the rank of $\boldsymbol{\Gamma}$ is $N - v_o$, where v_o denotes the algebraic degeneracy of the eigenvalue $\lambda_o = 0$ we obtain for the asymptotic probability, p_{as}, using well-known properties of the Jordan matrices [27]:

$$\mathbf{p}_{as} = \mathbf{H}^{-1}\begin{pmatrix} \mathbb{1}_{v_o} & 0 \\ 0 & 0 \end{pmatrix}\mathbf{H}\mathbf{p}(0). \tag{3.14}$$

The statistical properties are not affected if the N states are renumbered so that $\boldsymbol{\Gamma}$ becomes the following reducible matrix $\boldsymbol{\Gamma}'$

$$\boldsymbol{\Gamma}' = \begin{pmatrix} \Gamma_1 & & 0 & -B_1 \\ & \ddots & & \vdots \\ & & \Gamma_{v_o} & -B_{v_o} \\ & 0 & & B \end{pmatrix}. \tag{3.15}$$

Here the stochastic submatrices $\boldsymbol{\Gamma}_i$, $i = 1, \ldots, v_o$, with m_i states represent the v_o disjunct ergodic classes and the residue of the q states in B

$$q = N - \sum_{i=1}^{v_o} m_i, \tag{3.16}$$

corresponds to all the states in the nonergodic classes. Each ergodic class has a positive definite ergodic probability $\mathbf{p}_{st}^{(i)}$ with

$$\boldsymbol{\Gamma}_i \mathbf{p}_{st}^{(i)} = 0, \qquad \sum_{k=1}^{m_i} p_{st}^{(i)}(k) = 1, \quad i = 1, \ldots, v_o. \tag{3.17}$$

The special set of linear independent probabilities $\{p_{st}^{\mu}\}$ in equation (3.12) is then given by the 'extremal probabilities' $\{p_{st}^{\mu}\}$

$$p_{st}^{\mu}(i)\begin{cases} p_{st}^{\mu}(i) > 0, & \text{if } i \in C_{\mu}^{erg}, \\ 0, & \text{otherwise}. \end{cases} \tag{3.18}$$

Let $\mathbf{H}$ be decomposed in rows of left eigenvectors, $\mathbf{h}_i$, and $\mathbf{H}^{-1}$ into columns of right eigenvectors, g_j, of $\boldsymbol{\Gamma}'$ so that

$$\mathbf{h}_i \mathbf{g}_j = \delta_{ij}; \tag{3.19}$$

then we get with equation (3.14) for the asymptotic probability the useful decomposition

$$\mathbf{p}_{as} = \sum_{\mu=1}^{v_o} \omega_\mu \mathbf{p}_{st}^{\mu} \tag{3.20}$$

with

$$0 \le \omega_\mu = \mathbf{h}_\mu \mathbf{p}(0) \le 1; \qquad \sum_{\mu=1}^{v_o} \omega_\mu = 1. \tag{3.21}$$

The eigenvectors $\mathbf{h}_\mu$, $\mu = 1, \ldots v_o$ correspond to left eigenvectors of $\boldsymbol{\Gamma}'$ with eigenvalue $\lambda_\mu = 0$. The form of equation (3.20) can be interpreted as follows. The term ω_μ consists of part of the initial probability $\mathbf{p}(0)$ of preparation which corresponds to the *ergodic class* C_{μ}^{erg} *plus the part* of $\mathbf{p}(0)$ which becomes scattered from the q nonergodic states into the ergodic class C_{μ}^{erg}. (Note that from equation (3.19): $h_\mu(i) = 1$, if

$i \in C_\mu^{\text{erg}}$ and $h_\mu(i) = 0$, if $i \in \{\Sigma - C_\mu^{\text{erg}} - B\}$, $\mu = 1, \ldots, \nu_o$). If $\nu_o = 1$, p_{as} is the unique ergodic probability with $\omega_1 = 1$. Further, different initial probabilities with the same weighting factors $\{\omega_\mu\}$ for the ergodic classes $\{C_\mu^{\text{erg}}\}$ approach each other in function of time.

4. Symmetries of stochastic processes

There are two kinds of symmetries for stochastic processes, the consequences of which are worthwhile to study in greater detail. They are symmetry transformations in the state space Σ as well as symmetry conditions for the joint probability of a stationary Markov process by interchanging the time arguments (generalized detailed balance). Let us consider a transformation S: $\hat{\mathbf{x}} = S\mathbf{x}$ in state space Σ, e.g. a kind of a general coordinate transformation. All relations expressing physical properties (e.g., the probability flux or a thermodynamic potential) should be manifestly independent of the coordinates used. Covariant formulations of physical properties of continuous Markov processes have recently been given [31]. But stochastic equations, as the master equation, will change in general under such transformations. We consider a transformation S in state space which conserves state space volume, so that the Jacobian $J(\hat{\mathbf{x}}, \mathbf{x}) = \|\partial\hat{\mathbf{x}}/\partial\mathbf{x}\|$ equals unity. Further we assume that the *inverse transformation* of S also exists.[6]) The transformation induces then a transformation in function space Π by a linear operator O_S (transformation operator) according to

$$\hat{p}(\mathbf{x}t) = [O_S p(t)]_{\mathbf{x}} = p(S^{-1}\mathbf{x}t). \tag{4.1}$$

It must be emphasized that the operator acts upon the state space variables $\mathbf{x}$ and not on the argument of $p(\mathbf{x}t)$. Thus we mean $O_R[O_S^{-1}p]_{\mathbf{x}} = p(SR^{-1}\mathbf{x}) \neq p(R^{-1}S\mathbf{x})$. Such a transformation yields with respect to the generator of a time-homogeneous Markov process the relation

$$\hat{\Gamma} = O_S \Gamma O_S^{-1} \tag{4.2}$$

or

$$\hat{\Gamma}(\mathbf{x}, \mathbf{y}) = \Gamma(S^{-1}\mathbf{x}, S^{-1}\mathbf{y}). \tag{4.3}$$

We define a *symmetry transformation* S to a given stochastic generator as such that the form of the generator is the same in the old and the new coordinate system. Hence we obtain

$$\Gamma O_S = O_S \Gamma, \tag{4.4}$$

$$\Gamma(\mathbf{x}, \mathbf{y}) = \Gamma(S^{-1}\mathbf{x}, S^{-1}\mathbf{y}). \tag{4.5}$$

If $\{S\}$ is the set of all symmetry transformations of a stochastic generator Γ, the set $\{O_S\}$[7]) forms a group G, called the *symmetry group* G of the stochastic process. This follows trivially from the fact that S^{-1} exists and if Γ is invariant in $\hat{\mathbf{x}}$ then obviously Γ is invariant under $\hat{\mathbf{x}}' = S^{-1}\hat{\mathbf{x}} = \mathbf{x}$.

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[6]) In this case $\mathbf{y} = S\mathbf{x}$ has no multiple roots, so that $\hat{p}(\mathbf{y}) = p(\mathbf{x})/|\|\partial\mathbf{y}/\partial\mathbf{x}\||$. In general we would have $\hat{p}(\mathbf{y}) = \sum_{i=1}^{n} p(\mathbf{x}^{(i)})/|J(\mathbf{y}^{(i)}, \mathbf{x}^{(i)})|$, where $i = 1 \ldots n$ stands for the n real solutions of $\mathbf{y}(\mathbf{x}) = S\mathbf{x}$.

[7]) Note that a representation for O_S cannot be chosen in general to be unitary.

For stationary Markov processes the symmetry group G yields some important consequences. If we deal with an ergodic process, i.e. the stationary probability is ergodic, we obtain

$$p_{as}(\mathbf{x}) = [O_S p_{as}]_{\mathbf{x}}, \quad \forall S \in G. \tag{4.6}$$

This follows from the fact that p_{as} belongs to the eigenvector of the nondegenerate eigenvalue $\lambda = 0$ of Γ and has to be nodeless. If we decompose the state space Σ into ergodic classes $\{C_\mu^{erg}\}$ and rest region B, by using the principles in Section 3, the following statement holds: the ergodic classes $\{C_\mu^{erg}\}$ (or regions) can be grouped into *stars* $\{S_i\}$ of symmetry related classes which are transformed into each other under the elements of the symmetry group G of $\mathbf{x}(\mathbf{t})$. Each extremal probability, p_{st}^μ, in an ergodic class C_μ^{erg} is invariant under the *small group* G_μ transforming C_μ^{erg} into itself. The detailed proof for this theorem is given elsewhere [5]. If the stochastic generator depends on external parameters $\boldsymbol{\lambda}$, we always may assume that a change of $\boldsymbol{\lambda}$ does not change the symmetry group. Therefore only the details of stochastic properties can depend on the parameters $\boldsymbol{\lambda}$, but the global symmetry G is retained. However the specific symmetries of the states in state space are not retained (symmetry breaking instabilities) [1, 3]. For example, in a laser system all states with zero amplitude have a complete phase angle rotation invariance, the finite amplitude has a fixed, though arbitrary, phase.

From equation (4.5) we get for finite times τ, assuming a unique solution to the forward and backward equation for the stationary conditional probability,

$$R(\mathbf{x}, \tau \mid \mathbf{y}, o) = R(S\mathbf{x}, \tau \mid S\mathbf{y}, o), \quad \forall S \in G. \tag{4.7}$$

Hence, we have for the multivariate stationary probability of an ergodic process with equations (2.13, 4.6)

$$p^{(n)}(\mathbf{x}_1 t_1, \ldots, \mathbf{x}_n t_n) = p^{(n)}(S\mathbf{x}_1 t_1, \ldots, S\mathbf{x}_n t_n), \quad \forall S \in G. \tag{4.8}$$

Moreover, the stationary correlation of a set of state functions $\{\phi_1(\mathbf{x}), \ldots, \phi_n(\mathbf{x})\}$ fulfills the symmetry relation

$$\langle \phi_1(\mathbf{x}(t_1)) \ldots \phi_n(\mathbf{x}_n(t_n)) \rangle = \langle \bar{\phi}_n(\mathbf{x}_1(t_1)) \ldots \bar{\phi}_n(\mathbf{x}_n(t_n)) \rangle, \quad \forall S \in G, \tag{4.9}$$

where

$$\bar{\phi}(\mathbf{x}(t)) = \phi(S\mathbf{x}(t)). \tag{4.10}$$

Sometimes, the stationary Markov processes obey a certain symmetry which involves an interchanging of time-arguments in the joint-probabilities. Let T again denote a volume preserving state space transformation which is *not* necessarily a symmetry transformation. We define the *generalized detailed balance symmetry* by the following requirement for the stationary joint-probability $p^{(2)}$ of the process under consideration

$$p^{(2)}(\mathbf{x}\tau; \mathbf{y}o; \boldsymbol{\lambda}) = p^{(2)}(T\mathbf{y}\tau; T\mathbf{x}(o); T\lambda). \tag{4.11}$$

$\boldsymbol{\lambda} = \{\lambda_1 \ldots \lambda_m\}$ is a set of external parameters such as a magnetic field or an electric field. If T denotes the time-reversal operation S_0, equation (4.11) is the usual detailed balance symmetry [1, 3, 31–34]. The symmetry condition in equation (4.11) cannot be expected to hold in general for open systems, but there exists a number of interesting cases of non-equilibrium systems where such a symmetry condition holds accidently [1, 3]. This may be due to the well chosen coarse-graining in state space and time yielding a special structure of the generator Γ. Equation (4.11) is fulfilled further for $T = TS$, where S(or S^{-1}) belongs to a symmetry transformation $S \in G$ of the stationary ergodic Markov process. We then obtain

$$\begin{aligned} p^{(2)}(\mathbf{x}\tau;\mathbf{y}o;\boldsymbol{\lambda}) &= p^{(2)}(S\mathbf{x}\tau;S\mathbf{y}o;S\lambda) \\ &= p^{(2)}(T\mathbf{y},\tau;T\mathbf{x}o;T\boldsymbol{\lambda}) \\ &= p^{(2)}(TS\mathbf{y},\tau;TS\mathbf{x}o;TS\boldsymbol{\lambda}) \quad \text{etc.,} \end{aligned} \tag{4.12}$$

yielding a minimal region in the product space $\Sigma \times \Sigma$ from where the value for the joint-probability $p^{(2)}(\mathbf{x}t + \tau;\mathbf{y}t) \in \Pi(\Sigma \times \Sigma) \equiv \Pi^2$ can be extended to the full space.

Integrating equation (4.11) over $\mathbf{x}$ we obtain a symmetry condition for $p_{st}(\mathbf{y},\boldsymbol{\lambda})$

$$p_{st}(\mathbf{y},\boldsymbol{\lambda}) = p_{st}(T\mathbf{y},T\boldsymbol{\lambda}). \tag{4.13}$$

In contrast to equation (4.6) this symmetry condition holds for any volume preserving state space transformation T (not necessarily a symmetry transformation S) and *non-ergodic* stationary Markov processes. For the stationary n-time joint probability $p^{(n)} \in \Pi^n$, we obtain with use of the stationary condition:

$$\begin{aligned} p^{(2)}(\mathbf{x}_1 t_1;\mathbf{x}_2 t_2;\boldsymbol{\lambda}) &= p^{(2)}(T\mathbf{x}_2 t_1;T\mathbf{x}_1 t_2;T\boldsymbol{\lambda}) \\ &= p^{(2)}(T\mathbf{x}_1 - t_1;T\mathbf{x}_2 - t_2;T\boldsymbol{\lambda}), \end{aligned} \tag{4.14}$$

for the time set $t_1 \leq \cdots \leq t_n$ the important relation:

$$\begin{aligned} p^{(n)}(\mathbf{x}_1 t_1,\ldots,\mathbf{x}_n t_n;\boldsymbol{\lambda}) &= R(T\mathbf{x}_{n-1} - t_{n-1} \mid T\mathbf{x}_n - t_n;T\boldsymbol{\lambda}) \\ &\quad \times \frac{p_{st}(T\mathbf{x}_n,T\boldsymbol{\lambda})}{p_{st}(T\mathbf{x}_{n-1},T\boldsymbol{\lambda})} p^{(n-1)}(\mathbf{x}_1 t_1 \ldots \mathbf{x}_{n-1} t_{n-1}) \\ &= p^{(n)}(T\mathbf{x}_n - t_n,\ldots,T\mathbf{x}_1 - t_1,T\boldsymbol{\lambda}). \end{aligned} \tag{4.15}$$

Thereby we have made extensive use of the Markov property in equations (2.11–2.13). For the stationary correlation of n state functions $\{\phi_1 \ldots \phi_n\}$ we have with equation (4.15) the relationship

$$\langle \phi_1(\mathbf{x}t_1)\ldots\phi_n(\mathbf{x}t_n)\rangle_{\lambda} = \langle \phi_n(T^{-1}\mathbf{x},-t_n)\ldots\phi_1(T^{-1}\mathbf{x},-t_1)\rangle_{T\lambda}. \tag{4.16}$$

For the following we introduce the transformed generator $\bar{\Gamma}(\boldsymbol{\lambda})$ with the kernel

$$\bar{\Gamma}(\mathbf{x},\mathbf{y};\boldsymbol{\lambda}) = p_{st}^{-1/2}(\mathbf{x};\boldsymbol{\lambda})\Gamma(\mathbf{x},\mathbf{y};\boldsymbol{\lambda})p_{st}^{1/2}(\mathbf{y};\boldsymbol{\lambda}). \tag{4.17}$$

With $\bar{p}(t) = p_{st}^{-1/2}p(t)$, the operator $\bar{\Gamma}$ is the generator for the master equation

$$\frac{d}{dt}\bar{p}(t;\boldsymbol{\lambda}) = \bar{\Gamma}(\boldsymbol{\lambda})\bar{p}(t;\boldsymbol{\lambda}). \tag{4.18}$$

Taking the derivative with respect to τ on both sides of equation (4.11) and putting $\tau = 0^+$ we obtain with equation (2.4), a second version of the generalized detailed balance condition

$$\Gamma(\mathbf{x},\mathbf{y};\boldsymbol{\lambda})p_{st}(\mathbf{y};\boldsymbol{\lambda}) = \Gamma(T\mathbf{y},T\mathbf{x};T\boldsymbol{\lambda})p_{st}(\mathbf{x},\boldsymbol{\lambda}). \tag{4.19}$$

Hence, a *necessary and sufficient operator condition* for the generalized detailed balance symmetry is then given by

$$p_{st}(\mathbf{x},\boldsymbol{\lambda}) = p_{st}(T\mathbf{x},T\boldsymbol{\lambda}), \tag{4.20}$$

operator equation

$$\Gamma(\lambda) = \Gamma^+(T\lambda). \quad \text{or} \quad O_T^{-1}\,\bar{\Gamma}^+(\lambda)\,O_T = \bar{\Gamma}(\lambda) \tag{4.21}$$

In equation (4.21) $\Gamma^+(T\lambda)$ denotes the transpose of the operator Γ with kernel $\Gamma^+(T\mathbf{x}, T\mathbf{y}; T\lambda) = \Gamma(T\mathbf{y}, T\mathbf{x}; T\lambda)$.

For a general time-homogeneous Markov process the dissipative generator $\Gamma(\lambda)$ may have 'right' eigenfunctions $\psi_\nu(\mathbf{x}, \lambda)$ with eigenvalues λ_ν and Re $\lambda_\nu \leq 0$

$$[\Gamma(\lambda)\psi_\nu(\lambda)]_{\mathbf{x}} = \lambda_\nu\psi_\nu(\mathbf{x};\lambda), \tag{4.22}$$

and 'left' eigenfunctions $\hat{\psi}_\nu(\mathbf{x}, \lambda)$

$$[\Gamma^+(\lambda)\hat{\psi}_\nu(\lambda)]_{\mathbf{x}} = \lambda_\nu^*\hat{\psi}_\nu(\mathbf{x};\lambda). \tag{4.23}$$

The notation (*) in equation (4.23) denotes the complex conjugation. Then the sets $\{\psi_\nu\}$ and $\{\hat{\psi}_\nu\}$ form a biorthogonal set [35]

$$\int \hat{\psi}_\mu^*(\mathbf{x};\lambda)\psi_\nu(\mathbf{x};\lambda)\,d\mathbf{x} = \delta_{\mu\nu}. \tag{4.24}$$

Next we assume that the eigenfunctions $\{\hat{\psi}_\nu\}$ and $\{\psi_\nu\}$ form a *complete* biorthogonal set

$$\mathop{\sum\!\!\!\!\!\!\int}_\nu \hat{\psi}_\nu^*(\mathbf{y};\lambda)\psi_\nu(\mathbf{x};\lambda)\,d\nu = \delta(\mathbf{x} - \mathbf{y}). \tag{4.25}$$

For the propagator $R(\tau)$ of the general time-homogeneous Markov process we obtain with equations (2.9, 4.18, 4.25) the expression

$$R(\mathbf{x}\tau \mid \mathbf{y}o;\lambda) = \left(\frac{p_{st}(\mathbf{x}, \lambda)}{p_{st}(\mathbf{y}, \lambda)}\right)^{1/2} \mathop{\sum\!\!\!\!\!\!\int}_\nu \hat{\psi}_\nu^*(\mathbf{y};\lambda)\psi_\nu(\mathbf{x};\lambda)\exp\lambda_\nu\tau\,d\nu, \quad \tau \geq 0. \tag{4.26}$$

In presence of a generalized detailed balance symmetry the calculation of the left eigenfunction $\{\hat{\psi}_\nu\}$ becomes rather simplified. From equation (4.21) we have

$$[\Gamma(T^{-1}\lambda)\psi_\nu(T^{-1}\lambda)]_{T^{-1}\mathbf{x}} = \lambda_\nu\psi_\nu(T^{-1}\mathbf{x}, T^{-1}\lambda) = [\Gamma^+(\lambda)\psi_\nu(T^{-1}\lambda)]_{\mathbf{x}}, \tag{4.27}$$

so that

$$\hat{\psi}_\nu^*(\mathbf{x}, \lambda) = \psi_\nu(T^{-1}\mathbf{x}, T^{-1}\lambda). \tag{4.28}$$

If we decompose the generator Γ into a symmetric part $\Gamma_S = \frac{1}{2}[\Gamma + \Gamma^+]$ and a skew-symmetric part $\Gamma_A = \frac{1}{2}[\Gamma - \Gamma^+]$, the calculation of the left eigenfunction $\hat{\psi}_\nu(\mathbf{x}\lambda)$ of Γ^+ becomes even more simplified in cases where Γ_S and Γ_A commute. Let ψ_ν denote an eigenfunction of Γ, so that we have

$$\Gamma_S\psi_\nu = (\mathrm{Re}\,\lambda_\nu)\psi_\nu, \tag{4.29}$$

and

$$\Gamma_A\psi_\nu = i(\mathrm{Im}\,\lambda_\nu)\psi_\nu. \tag{4.30}$$

It follows then from equations (4.23) and (4.28), that

$$\psi_\nu(T^{-1}\mathbf{x};T^{-1}\lambda) = \psi_\nu^*(\mathbf{x}, \lambda). \tag{4.31}$$

For the propagator, $R(\tau)$, we find by use of equation (4.28)

$$R(\mathbf{x}\tau \mid \mathbf{y}o, \lambda) = \left(\frac{p_{st}(\mathbf{x}, \lambda)}{p_{st}(\mathbf{y}, \lambda)}\right)^{1/2} \mathop{\sum\!\!\!\!\!\!\int}_\nu d\nu\psi_\nu(T^{-1}\mathbf{y}, T^{-1}\lambda)\psi_\nu(\mathbf{x}, \lambda)\exp\lambda_\nu\tau, \quad \tau \geq 0, \tag{4.32}$$

and for the stationary joint-probability $p^{(2)}$ the relation

$$p^{(2)}(\mathbf{x}, \tau; \mathbf{y}; o; \boldsymbol{\lambda}) = (p_{st}(\mathbf{x}, \boldsymbol{\lambda}) p_{st}(\mathbf{y}, \boldsymbol{\lambda}))^{1/2} \sum\!\!\!\!\!\!\int_\nu d\nu \hat{\psi}_\nu(T^{-1}\mathbf{y}, T^{-1}\boldsymbol{\lambda}) \psi_\nu(\mathbf{x}, \boldsymbol{\lambda}) \exp \lambda_\nu \tau, \quad \tau \geq 0. \tag{4.33}$$

For $\tau < 0$, we obtain, using the stationary condition (equation (4.14)):

$$p^{(2)}(\mathbf{x}, \tau; \mathbf{y}; o; \boldsymbol{\lambda}) = (p_{st}(\mathbf{x}, \boldsymbol{\lambda}) p_{st}(\mathbf{y}, \boldsymbol{\lambda}))^{1/2} \sum\!\!\!\!\!\!\int_\nu d\nu \hat{\psi}_\nu(T^{-1}\mathbf{x}, T^{-1}\boldsymbol{\lambda}) \psi_\nu(\mathbf{y}, \boldsymbol{\lambda}) \exp \lambda_\nu |\tau|. \tag{4.34}$$

Further, if $\mathbf{y} = T^{-1}\mathbf{y}$, $\boldsymbol{\lambda} = T^{-1}\boldsymbol{\lambda}$, i.e. we deal with a *strong* generalized detailed balance condition, the generator Γ becomes self-adjoint such that $0 \geq \lambda_\nu \in \mathbb{R}$, and the left eigenfunctions can be chosen to be $\hat{\psi}_\nu(\mathbf{x}, \boldsymbol{\lambda}) = \psi_\nu(\mathbf{x}, \boldsymbol{\lambda}) \in \mathbb{R}$. As a consequence, equations (4.33–4.34) for $p^{(2)}$ read in closed form

$$p^{(2)}(\mathbf{x}\tau, \mathbf{y}o; \boldsymbol{\lambda}) = (p_{st}(\mathbf{x}, \boldsymbol{\lambda}) p_{st}(\mathbf{y}, \boldsymbol{\lambda}))^{1/2} \sum\!\!\!\!\!\!\int_\nu d\nu \psi_\nu(\mathbf{y}, \boldsymbol{\lambda}) \psi_\nu(\mathbf{x}, \boldsymbol{\lambda}) \exp \lambda_\nu |\tau|. \tag{4.35}$$

All the relations discussed so far hold for general regular transformations T obeying equation (4.11). The property of volume preserving was only introduced for simplicity. It is easy to write all relations in terms of a general Jacobian $|J(\mathbf{y}, \mathbf{x})| \neq 1$. Also, it is self evident that in the special case of a strong detailed balance the symmetry group G can be advantageously studied in terms of the symmetric generator $\bar{\Gamma}$.

Finally, we consider operators T_0 which fulfill equation (4.11) and further:

$$T_0^2 = \mathbb{1}, \tag{4.36}$$

$$T_0 \lambda_i = \sum_j \alpha_{ij} \lambda_j, \tag{4.37}$$

$$T_0 x_i = \sum_j r_{ij} x_j. \tag{4.38}$$

By choosing the variables $\mathbf{x}$ and the external parameters appropriately we can always achieve $\boldsymbol{\alpha}$ and $\mathbf{r}$ to be diagonal with eigenvalues $\varepsilon_i = \pm 1$ (see equation (4.36)). In the following we speak of the parity, ε_i, for the variable x_i under the transformation T_0. As an example, in Table 1 we study the transformation behaviour of physical variables under the three different transformations T_0:

S_0: time reversal symmetry
R_0: inversion, or image symmetry
I_0: total inversion $I_0 = S_0 R_0$.

Most relations discussed above then simplify considerably. For example, the correlation function $S_{ij}(t)$ of two random variables fulfills (equation (4.16)):

$$S_{ij}(\tau) = \langle x_i(t) x_i(0) \rangle = \varepsilon_i \varepsilon_j S_{ji}(\tau). \tag{4.39}$$

Note, if equation (4.11) is fulfilled for two transformations of the set $\{S_0, R_0, I_0\}$, equation (4.11) is fulfilled by use of equation (4.12) for all three transformations $\{S_0, R_0, I_0\}$. In the case of the Fokker–Planck equation, equation (2.25), the operator condition in equation (4.21):

$$p_{st}(\mathbf{x}, \boldsymbol{\lambda}) = p_{st}(\hat{\mathbf{x}}, \hat{\boldsymbol{\lambda}}), \tag{4.40}$$

$$\Gamma_{FP}(\mathbf{x}, \boldsymbol{\lambda}) = \Gamma^+_{FP}(\hat{\mathbf{x}}, \hat{\boldsymbol{\lambda}}), \tag{4.41}$$

operation	charge mass	magnetic pole strength	position	velocity current	spin density	angular momentum	electric field	magnetic field
S_0	1	−1	1	−1	−1	−1	1	−1
R_0	1	−1	−1	−1	1	1	−1	1
I_0	1	1	−1	1	−1	−1	−1	−1

Table 1
Transformation behaviour, ε_i, of physical quantities with respect to time reversal S_0, inversion R_0 and total inversion $I_0 = S_0 R_0$.

where

$$\hat{\mathbf{x}} = \{\varepsilon_1 x_1, \ldots, \varepsilon_n x_n\}, \tag{4.42}$$

can be written in a more adequate form by introducing the following quantities:

$$a_i^{\pm}(\mathbf{x}, \boldsymbol{\lambda}) = \tfrac{1}{2}[a_i(\mathbf{x}, \boldsymbol{\lambda}) \pm \varepsilon_i a_i(\hat{\mathbf{x}}, \hat{\boldsymbol{\lambda}})], \tag{4.43}$$

so that

$$a_i^{\pm}(\mathbf{x}, \boldsymbol{\lambda}) = \pm\varepsilon_i a_i^{\pm}(\hat{\mathbf{x}}, \hat{\boldsymbol{\lambda}}), \tag{4.44}$$

and

$$\mathbf{S}^-(\mathbf{x}, \boldsymbol{\lambda}) = \mathbf{a}^-(\mathbf{x}, \boldsymbol{\lambda}) p_{st}(\mathbf{x}, \boldsymbol{\lambda}), \tag{4.45}$$

$$\mathbf{S}^+(\mathbf{x}, \boldsymbol{\lambda}) = \mathbf{a}^+(\mathbf{x}, \boldsymbol{\lambda}) p_{st}(\mathbf{x}, \boldsymbol{\lambda}) - \boldsymbol{\nabla}\cdot(\mathbf{D}(\mathbf{x}, \boldsymbol{\lambda}) p_{st}(\mathbf{x}, \boldsymbol{\lambda})). \tag{4.46}$$

Following the procedure of Risken, where $T_0 = S_0$ is considered [33], we obtain for *any* transformation T_0 obeying equation (4.11) for the necessary and sufficient conditions of detailed balance the so called potential conditions[8]) [1, 3, 31–34]

$$D_{ij}(\mathbf{x}, \boldsymbol{\lambda}) = \varepsilon_i \varepsilon_j D_{ij}(\hat{\mathbf{x}}, \hat{\boldsymbol{\lambda}}), \tag{4.47}$$

$$\mathbf{S}^+(\mathbf{x}, \boldsymbol{\lambda}) = \mathbf{0}. \tag{4.48}$$

$$\boldsymbol{\nabla}\cdot\mathbf{S}^-(\mathbf{x}, \boldsymbol{\lambda}) = 0. \tag{4.49}$$

If the diffusion matrix $\mathbf{D}$ possesses an inverse, equation (4.48) requires

$$-\frac{\partial \ln p_{st}(\mathbf{x}, \boldsymbol{\lambda})}{\partial x_i} = \sum_k D_{ik}^{-1}(\mathbf{x}, \boldsymbol{\lambda}) \left(\sum_l \frac{\partial D_{kl}(\mathbf{x}, \boldsymbol{\lambda})}{\partial x_l} - a_k^+(\mathbf{x}, \boldsymbol{\lambda}) \right), \tag{4.50}$$

[8]) A covariant formulation of these potential conditions has been discussed recently by Graham [31].

from which $p_{st}(\mathbf{x}, \boldsymbol{\lambda})$ is obtained by quadratures. Furthermore, if static fields $\{\boldsymbol{\lambda}\}$ are applied, such that $a_i^+(\mathbf{x}, \boldsymbol{\lambda}) = a_i^+(\mathbf{x}) + \lambda_i$, $\forall i$, and they restore the generalized detailed balance symmetry, we obtain in the case of **x**-independent diffusion coefficients for the stationary probability

$$p_{st}(\mathbf{x}, \boldsymbol{\lambda}) = \text{const}\, p_{st}(\mathbf{x}, \boldsymbol{\lambda} = \mathbf{0}) \exp \sum_{i,j} D_{ij}^{-1} x_j \lambda_j. \tag{4.51}$$

Note that $p_{st}(\mathbf{x}, \boldsymbol{\lambda} = \mathbf{0})$ obtained from equation (4.50) is, in general, non-Gaussian. The result of equation (4.51) allows the calculation of the *static response* to all orders.

Equation (4.50) shows that in the presence of a general detailed balance condition the stationary probability may be determined explicitly. The symmetry of the generalized detailed balance yields in equations (4.43–4.45) additional information not needed for the solution of the stationary probability. Hence, the study of potential conditions which yield the minimal necessary and sufficient information needed for the construction of the stationary probability is very desirable. Finally, we mention that the results obtained in this paper can be generalized to the case of functional master equations.

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REFERENCES

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[1] H. HAKEN, Rev. Mod. Phys. *47*, 67 (1975).
[2] A. NITZAN, P. ORTOLEVA, J. DEUTCH and J. ROSS, J. Chem. Phys. *61*, 1056 (1974).
[3] R. GRAHAM, Springer Tracts in Modern Physics *66*, 1 (Springer, New York 1973).
[4] F. HAAKE, Springer Tracts in Modern Physics *66*, 98 (Springer, New York 1973).
[5] P. HÄNGGI and H. THOMAS, Physics Reports, to be published.
[6] W. FELLER, *Introduction to Probability and its Application*, Vols. I and II (John Wiley, New York 1966).
[7] J. L. DOOB, *Stochastic Processes*, Chap. VI (John Wiley, New York 1953).
[8] I. I. GIHMAN, A. V. SKOROHOD, *The Theory of Stochastic Processes*, Vol. II (Springer, Berlin 1975).
[9] A. IOSIFESCU and P. TĂUTU, *Stochastic Processes and its Application in Biology and Medicine*, Vol. I (Springer, Berlin 1973).
[10] G. E. H. REUTER, Mathematika *14*, 56 (1967).
[11] H. A. KRAMERS, Physica *7*, 284 (1940).
[12] J. E. MOYAL, J. Roy. Stat. Soc. *B11*, 150 (1949).
[13] R. F. PAWULA, Phys. Rev. *162*, 186 (1967).
[14] I. I. GIHMAN and A. V. SKOROHOD, *Stochastic Differential Equations* (Springer, Berlin 1972).
[15] H. P. MCKEAN, *Stochastic Integrals* (Academic Press, New York 1969).
[16] E. J. MCSHANE, *Stochastic Calculus and Stochastic Models* (Academic Press, New York 1974).
[17] A. FRIEDMAN, *Stochastic Differential Equations and Applications*, Vols. I and II (Academic Press, New York 1976).
[18] R. L. STRATONOVICH, SIAM J. Contr. *A2*, No. 1 (196[illegible]).
[19] P. HÄNGGI and H. THOMAS, Z. Phys. *B22*, 295 (1975).
[20] E. NELSON, J. Math. Phys. *5*, 332 (1964).

[21] K. Yosida, *Functional Analysis* (Springer, Berlin 1972).
[22] J. Premanad, Phys. Rev. *138B*, 1320 (1965).
[23] W. Ledermann, Proc. Cambr. Phil. Soc. *46*, 581 (1950).
[24] W. Ledermann and G. E. H. Reuter, Phil. Trans. Roy. Soc. *A246*, 333 (1954).
[25] S. Gerschgorin, Isv. Akad. Nauk. SSSR Ser. fiz-mat. *6*, 749 (1931).
[26] O. Taussky, Amer. Math. Mon. *56*, 672 (1949).
[27] D. R. Cox and H. D. Miller, *Theory of Stochastic Processes*, p. 120 (Methuen, London 1965).
[28] A. Papoulis, *Probability, Random Variables and Stochastic Processes*, Chap. IX (McGraw-Hill, New York 1965).
[29] J. L. Lebowitz and P. G. Bergman, Ann. Phys. *1*, 1 (1957).
[30] D. A. Freedman, Ann. Math. Statist. *38*, 1552 (1967).
[31] R. Graham, Z. Phys. *B26*, 397 (1977).
[32] R. Graham and H. Haken, Z. Phys. *245*, 141 (1971).
[33] H. Risken, Z. Phys. *251*, 231 (1972).
[34] C. P. Enz, Lecture Notes in Physics, *54*, 79 (1976).
[35] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics*, pp. 884–886 (McGraw-Hill, New York 1953).