Stochastic Nonlinear Systems

in Physics, Chemistry, and Biology

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L. Arnold and R. Lefever

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Preface

This book contains the invited papers of the interdisciplinary workshop on "Stochastic Nonlinear Systems in Physics, Chemistry and Biology" held at the Center for Interdisciplinary Research (ZIF), University of Bielefeld, West Germany, October 5-11, 1980.

The workshop brought some 25 physicists, chemists, and biologists - who deal with stochastic phenomena - and about an equal number of mathematicians - who are experts in the theory of stochastic processes - together.

The Scientific Commitee consisted of L. Arnold (Bremen), A. Dress (Bielefeld), W. Horsthemke (Brussels), T. Kurtz (Madison), R. Lefever (Brussels), G. Nicolis (Brussels), and V. Wihstutz (Bremen).

The main topics of the workshop were the transition from deterministic to stochastic behavior, external noise and noise induced transitions, internal fluctuations, phase transitions, and irreversible thermodynamics, and on the mathematical side, approximation of stochastic processes, qualitative theory of stochastic systems, and space-time processes.

The workshop was sponsored by ZIF, Bielefeld, and by the Universities of Bremen and Brussels. We would like to thank the staff of ZIF and H. Crauel and M. Ehrhardt (Bremen) for the perfect organization and their assistance. In addition, our thanks go to Professor H. Haken for having these Proceedings included in the Series in Synergetics.

Bremen and Brussels
December 1980

L. Arnold and R. Lefever

Contents

Part I

Introduction: From Deterministic to Stochastic Behavior

On the Foundations of Kinetic Theory

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Abstract

We discuss the problem of deriving an *exact* Markovian master equation from dynamics *without* resorting to approximation schemes such as the weak coupling limit, Boltzmann-Grad limit, etc. Mathematically, it is the problem of the existence of a suitable positivity preserving operator Λ such that the unitary group U_t induced from dynamics satisfies the intertwining relation

$$\Lambda U_t = W_t^* \Lambda \quad , \quad t \geqq 0$$

with the contraction semigroup W_t of a strongly irreversible stochastic Markov process. Two cases are of special interest: i) $\Lambda = P$ is a projection operator, ii) Λ has a densely defined inverse. Our recent work, which we summarize here, shows that the class of (classical) dynamical systems for which a suitable projection operator satisfying the above intertwining relation exists is identical with the class of K flows or K systems. As a corollary of our consideration it follows that the function $\int \hat{\rho}_t \ln \hat{\rho}_t d\mu$ with $\hat{\rho}_t$ denoting the coarse-grained distribution with respect to a K partition obtained from $\rho_t \equiv U_t\rho$ is a Boltzmann-type H function for K flows. This is not in contradiction with the time-reversal (velocity-inversion) symmetry of dynamical evolution as the suitably constructed projection operator or the Λ transformation are dynamics dependent and break the time reversal.

1. Introduction

The study of the possible connections that may exist between deterministic dynamics and probabilistic processes is of obvious importance for the foundation of nonequilibrium statistical mechanics. As it is well known, stochastic Markov processes provide suitable models to represent irreversible evolution admitting a Liapounov functional or H function. The important question, thus, is how the passage from deterministic dynamics to probabilistic Markov processes is to be achieved.

Our work described below shows that in the presence of suitable instability of motion, described by the condition of K flow, the dynamical evolution indeed becomes *similar* in a well-defined sense to the stochastic evolution of a Markov process.

Let us recall that the procedure for obtaining a Markovian master equation from dynamics usually starts with an initial "contraction of description" or coarse graining brought about by a projection operator P. The operation of "coarse graining" alone, however, generally leads to the so-called generalized master equation which is non-Markovian in character [1]. To obtain a Markovian evolution equation one needs to consider a special asymptotic limit (e.g., the weak coupling limit etc.). Thus, even when this program succeeds, the resulting master equation is only an approximation. To lay a more satisfactory foundation of nonequilibrium statistical mechanics it seems desirable to investigate the possibility of establishing *exact* Markovian master equations whose validity does not depend on sepcial approximation schemes. This paper summarizes our recent work in this direction [2-6]. We shall discuss the problem for classical dynamical systems. Our main result is that the class of dynamical systems for which an *exact* Markovian master equation follows from a suitable projection operation alone is not empty, but is precisely the class of so-called K flow. The condition of K flow is thus seen to play the same role in the foundation of nonequilibrium statistical mechanics as that of ergodicity in the foundation of equilibrium statistical mechanics.

Let us, however, mention that just as the method of replacing time average by ensemble average can be justified for a special class of functions on phase space even if the system as a whole is not ergodic, one may be able to derive a exact Markovian master equation for special subclass of initial distributions even if the system is not a K flow. But it is only for K flows that one can derive an exact master equation through a projection operator for all initial distribution functions in $L^2_\mu \cap L^1_\mu$.

2. Formulation of the Problem

Consider an abstract dynamical system (Γ, B, μ, T_t). Here Γ denotes the phase space of T_t the system equipped with a σ algebra of measurable subsets, T_t a group of measurable transformations mapping Γ onto itself and preserving the measure μ. For example, Γ could be the energy surface of a classical dynamical system, T_t the group of dynamical evolution and μ the invariant measure whose existence is assured by Liouville's theorem. For convenience we shall assume the measure μ to be normalized: $\mu(\Gamma) = 1$. As is well known, the evolution $\rho \to \rho_t$ of density functions under the given deterministic dynamics is described by the unitary group U_t induced by T_t

$$\rho_t(\omega) = (V_t\rho)(\omega) = (T_{-t}\omega) \quad .$$

The generator L of the unitary group U_t is called the Liouvillian operator of the system: $U_t = \exp(-itL)$. It is given by Poisson bracket with the Hamiltonian H:

$$L\rho = i[H,\rho]_{P.B.}$$

for Hamiltonian evolution.

On the other hand, stochastic Markov processes on the state space Γ, preserving μ, are associated with contraction semigroups of L^2_μ 8 . In fact, let $P(t,\omega,\Delta)$ denote the probability of transition from the point $\omega \in \Gamma$ to the region Δ in time t. Then the operators W_t defined by

$$(W_t f)(\omega) = \int f(\omega')P(t,\omega,d\omega')$$

form a contraction semigroup for $t \geq 0$. Moreover, W_t has the following properties:

i) W_t preserves positivity (i.e., $f \geq 0$ implies $W_t f \geq 0$ for $t \geq 0$),

ii) W_t .1. = 1.

The evolution of the distribution functions ρ under the Markov process is described now by the ajoint semigroup W_t^* which also preserves positivity since W_t does: $\rho_0 \to \rho_t = W_t^* \rho_0$. Since the measure μ is an invariant measure for the process (or equivalently the *microcanonical distribution function* 1 is the equilibrium state of the process) we also have

iii) $W_t^* \cdot 1 = 1$.

Every Markov process on Γ with stationary measure μ is thus associated with a contraction semigroup satisfying the conditions i-iii). Conversely, every contraction semigroup W_t on Γ satisfying the above conditions comes from a stochastic Markov process, the transition probabilities $P(t,\omega,\Delta)$ being given by

$$P(t,\omega,\Delta) = (W_t \varphi_\Delta)(\omega) \quad .$$

Here φ_Δ denotes the characteristic (or indicator) function of the set Δ.

In the following we are interested in a special class of Markov processes whose semigroups W_t satisfy [in addition to conditions i-iii)] the condition:

iv) $\| W_t^*\rho - 1\|^2$ decreases strictly monotonically to 0 as $t \to +\infty$; for all states $\rho \neq 1$ (i.e., for all nonnegative distribution functions with $\int \rho \, d\mu = 1$). This condition expresses the requirement that any initial distribution ρ tends strictly monotonically in time to the equilibrium distribution 1. For such processes the functional

$$\int_\Gamma \rho_t \log \rho_t d\mu \quad , \quad \rho_t = W_t^* \rho_0$$

and indeed any other convex functional of ρ_t is an H function. Such Markov processes thus provide the best possible model of irreversible evolution obeying the law of monotonic increase of entropy. Semigroups satisfying the conditions i-iv) will be called *strongly irreversible Markov semigroups*.

The problem before us is to determine the class of dynamical systems for which one can construct a bounded operator Λ having the following properties

i) Λ preserve positivity,

ii) $\Lambda 1 = 1$

iii) $\int_\Gamma \Lambda\rho \, d\mu = \int_\Gamma \rho \, d\mu$

iv) The dynamical group $U_t = \exp(-itL)$ satisfies the intertwining relation: $\Lambda U_t = W_t^* \Lambda$ (for $t \geq 0$) with a strongly irreversible Markov semigroup W_t.

We shall consider two cases:

First, Λ has a densely defined inverse Λ^{-1}. In this case Λ may be interpreted as defining a "change of representation" of dynamics $\rho_t = U_t\rho_0 \to \Lambda\rho_t = \tilde{\rho}_t$. Condition iv) then means that the evolution of transformed states obeys the master equation of the Markov process W_t. For dynamical systems admitting an invertible operator Λ satisfying conditions i-iv), the dynamical group U_t is similar to a strongly irreversible Markov semigroup $\Lambda U_t \Lambda^{-1} = W_t^*$ for $t \geq 0$.

Note that the demanded invertibility of Λ assures that the passage $\rho \to \Lambda\rho = \tilde{\rho}$ involves no "loss of information". Dynamical systems admitting such a Λ may, hence, be said to be *intrinsically random*.

The other case we consider is: Λ is a projection operator P. Such projection operators [i.e., projections P satisfying conditions i-iii), with Λ replaced by P] correspond to operations of "coarse graining". The existence of such a projection P satisfying the intertwinning relation iv) thus implies an *exact* Markovian master equation for the system which does not depend on special approximation schemes, but results solely from the projection operator P.

As described below, it is a remarkable fact that there is a rather general class of dynamical systems for which an exact master equation holds in this sense.

3. Dynamical Systems Admitting Exact Markovian Master Equations

A K flow is, by definition [9], an abstract dynamical system $(\Gamma, \mathcal{B}, \mu, T_t)$ for which there exists a distinguished (measurable) partition ξ_0 of the phase space into disjoint cells having the following properties

i) $\xi_t = T_t\xi_0 \geq \xi_s$ if $t \geq s$.

Here $T_t\xi_0 = \xi_t$ is the partition into which the original partition ξ_0 is transformed in time under the dynamical evolution. The notation $\xi_t \geq \xi_s$ signifies that the partition ξ_t is "finer" than ξ_s (i.e., every cell of ξ_t is entirely contained in one of the cells of ξ_s).

ii) The (least fine) partition $\bigvee_{t=-\infty}^{\infty}$ which is finer than each ξ_t, $-\infty < t < +\infty$ is the partition of the phase space into distinct phase points.

iii) The (finest) partition $\bigcap_{t=-\infty}^{\infty}\xi_t$ which is less fine than every ξ_t $-\infty < t < +\infty$ is a trivial partition consisting of a cell of measure 1.

A partition ξ_0 with the above-stated properties is called a K partition. Many systems of physical interest have been recently found to be K flows, for instance, the motion of hard spheres within a finite box [10], the geodesic flow on space of constant negative curvature [11], the Lorentz gas, and infinite ideal gas and hard rod systems, etc. Generally, a K partition consists of an uncountable number of cells, each of null μ measure. The notion of coarse graining with respect to a K partition cannot, therefore, be defined directly as the operation of taking averages over the cells of the partition. The appropriate extension of the usual concept of coarse graining is provided by the projection operator P_0 of $L^2\mu$ onto the subspace $L^2[a(\xi_0),\mu]$. Here $a(\xi_0)$ denotes the σ subalgebra of $\mathcal{B}$ consisting of only those measurable subsets of Γ that are unions of cells in ξ_0 and $L^2[a(\xi_0),\mu]$ is the subspace of all $f \in L^2\mu$ that are measurable with respect to $a(\xi_0)$. In fact, it is clear that for any nonnegative density function ρ the function $P_0\rho$ has the following characteristic properties of coarse graining distribution with respect to the partition

i) $P_0\rho = \hat{\rho} \geq 0$,

ii) $\int_\Gamma \hat{\rho}\, d\mu = \int_\Gamma \rho\, d\mu$,

iii) $\hat{\rho}$ being measurable with respect to $a(\xi_0)$, can only assume constant values on individual cells of ξ_0,

iv) $\int_\Delta \hat{\rho}\, d\mu = \int_\Delta \rho\, d\mu$
for any measurable Δ_0 that is a union of cells in ξ_0.

The (self-adjoint) projection operation P_0 of coarse graining with respect to a partition ξ_0 obviously preserves positivity and maps the constant function (microcanonical ensemble) onto itself. It is interesting that the converse is also true. For standard measure spaces $(\Gamma,\mathcal{B},\mu)$ with $\mu(\Gamma) = 1$ every self-adjoint projection operation P of $L^2\mu$ that preserves positivity and maps the constant function onto itself is the projection operator onto $L^2[a(\xi),\mu]$ for some measurable partition ξ of Γ. The operations of coarse graining may thus be identified with (self-adjoint) projection operators P satisfying

i) $f \geq 0 \Rightarrow Pf \geq 0$ and

ii) $P1 = 1$.

The following theorem tells that the condition of K flow is both necessary and sufficient for the existence of an operation of coarse graining that converts the dynamical evolution into that of a strongly irreversible stochastic Markov process.

4. Theorem 1

Suppose a dynamical system with induced unitary group U_t of dynamical evolution admits a positivity preserving projection P mapping the unit function 1 to itself such that

i) $PU_t\rho = PU_t\rho'$ for all $t \Rightarrow \rho = \rho'$, and

ii) $PU_t = W_t^*P$ for $t \geq 0$,

where W_t is a *strongly irreversible Markov semigroup* (see Sect.2 for definition). Then the dynamical system is necessarily a K flow. Conversely, ever K flow admits a positivity preserving projection {namely, the projection onto $L^2[a(\xi_0),\mu]$ with ξ_0 denoting a K partition} satisfying the conditions i) and ii) above.

Remark: Condition i) means that the coarse graining under consideration is sufficiently fine so that a knowledge of the coarse grained distribution $PU_t\rho$ during the entire history, both past and future, of the system's evolution is equivalent to a knowledge of the original distribution.

We shall not stop here for a proof of the theorem which may be found elsewhere, but let us mention an important corollary of this result.

5. Corrollary 2

For K flows the (negative) entropy functional

$$\Omega(\rho_t) = \int \hat{\rho}_t \log \hat{\rho}_t \, d\mu \quad , \quad \hat{\rho}_t = P_0 U_t \rho$$

with P_0 denoting the coarse graining projection operation with respect to a K partition, is a monotonically decreasing function (H function) of t which attains the fine-grained value $\int \rho \ln \rho \, d\mu$ at $t \to -\infty$ and the equilibrium value (0 due to our normalization of μ) at $t \to +\infty$.

This result follows immediately from theorem 1 because $\hat{\rho}_t = P_0U_t\rho = W_t^*P_0\rho = W_t^*\rho_0$ where W_t is the semigroup of a *strongly irreversible Markov process*. It is well-known that for such processes the functional Ω, and indeed any convex functional of $\hat{\rho}_t$, is an H function. Let us mention that this result has recently been obtained by Penrose and Goldstein by an independent argument [12].

Finally, let us mention that for K flow one cannot only construct a coarse graining operation that leads from the deterministic and reversible evolution U_t to that of a strongly irreversible stochastic process, but one can also construct an *invertible* and positivity preserving transformation Λ such that $\Lambda U_t \Lambda^{-1}$ is a strongly irreversible Markov semigroup for $t \geq 0$. In other terms, the unitary group U_t induced from every K flow is nonunitarily equivalent, through a positivity preserving similarity Λ, to the contraction semigroup of a stochastic Markov process.

A detailed discussion of this construction is described in our previous publications [4,5]. Let us only mention that the operator Λ establishing nonunitary equivalence between U_t and a stochastic Markov process W_t^* may be constructed as a *suitable* function of operator time T [3]

$$\Lambda = h(T) + P_{-\infty}$$

$$T = \int_{-\infty}^{+\infty} \lambda dF_\lambda \quad , \quad F_\lambda = U_\lambda P_0 U_\lambda^* - P_{-\infty} \quad .$$

Here P_0 denotes the projection of coarse graining with respect to the K partition ξ_0 and $P_{-\infty}$, the projection to the equilibrium ensemble. With Λ constructed as above, the functional

$$\int_\Gamma \tilde{\rho}_t \log \tilde{\rho}_t \, d\mu \quad , \quad \tilde{\rho}_t \equiv \Lambda U_t \rho$$

is again an H function.

6. Concluding Remarks

Let us emphasize that the possibility of obtaining an exact master equation from dynamics as discussed here comes from the existence of suitable *dynamics-dependent* operator Λ or P_0 that explicitly break the time-reversal (or velocity-inversion) symmetry. The necessity of considering such dynamics-dependent transformations for the passage from dynamics to irreversible evolution have been discussed in a previous publication [2]. This should be distinguished from the usual procedure of obtaining a master equation via a generalized master equation, where one starts with a projection that does not depend on dynamics and does not break the time-reversal symmetry. In fact, as well known, it is the approximation schemes (such as weak coupling limit) that breaks the time-reversal symmetry in the conventional approach.

To see explicitly the noninvariance of the projection P_0 under velocity inversion let us consider the operation of velocity inversion which, by definition, has the following properties

i) V preserves positivity,

ii) $V^2 = I$,

iii) $VU_t = U_{-t}V$.

Now, P_0 being the projection with respect to the K partition ξ_0, it is clear that $U_t P_0 U_t^* = P_t$ is the projection with respect to $T_t \xi_0$. The defining properties of ξ_0 (see Sect.2) translate into the following properties of P_t

i) $P_t \geq P_s$ if $t \geq S$,

ii) $\lim_{t \to \infty} P_t = I$, and

iii) $\lim_{t \to -\infty} P_t = P_{-\infty}$

the projection onto the equilibrium ensemble. Suppose now that P_0 is invariant under V, $VP_0V = P_0$. This would then imply that

$$P_t = U_tP_0U_t^* = U_tVP_0VU_t^* = VU_{-t}P_0U_{-t}^*V = VP_{-t}V \quad .$$

Since $P_t \geq P_0$ for $t \geq 0$ it follows that

$$P_{-t} = VP_tV \geq VP_0V = P_0 \quad \text{for} \quad t \geq 0 \quad .$$

Thus we have

$$P_t = U_tP_0U_t^* \geq P_0 \quad \text{for } \mathit{all} \text{ real } t$$

which is possible only if $P_0 = U_tP_0^{-1}U_t^*$ or P_0 commutes with U_t. This contradicts, however, the properties that $P_t \to I$, $t \to +\infty$ and $P_t \to P_{-\infty}$, $t \to -\infty$.

A variant of this argument shows also that no projection operator P (whether coming from a K partition or not) which commutes with velocity inversion V can yield an exact master equation, i.e., satisfy the relation $PU_t = W_t^*P$ (for $t \geq 0$) with a strongly irreversible Markov semigroup W_t.

Similar considerations show that the symmetry of velocity inversion is also broken by invertible transformation Λ. It fact if $V\Lambda V = \Lambda$ it would follow that together with $\Lambda U_t\Lambda^{-1}$ (for $t \geq 0$) the operation $V\Lambda U_t\Lambda^{-1}V = \Lambda U_{-t}\Lambda^{-1}$ also preserves positivity. However, $\Lambda U_{-t}\Lambda^{-1}$ is the inverse of $\Lambda U_t\Lambda^{-1}$ and they both can preserve positivity if and only if $\Lambda U_t\Lambda^{-1}$ is unitary [7]. This, however, contradicts the established fact [4,5] that, with Λ constructed as described in a previous section, $\Lambda U_t\Lambda^{-1}$ is a strongly irreversible Markov semigroup and hence nonunitary.

Finally, let us briefly show that the classical objection (such as those of Zermelo and Loschmidt) against the derivation of Boltzmann's H theorem does not apply to the H functions $\Omega(\rho_t)$ considered by us

$$\Omega(\rho_t) = \int_\Gamma \hat{\rho}_t \log \hat{\rho}_t \, d\mu$$

with

$$\hat{\rho}_t = P_0\rho_t \quad \text{or} \quad \Lambda\rho_t \quad , \quad \hat{\rho}_t = U_t\rho \quad .$$

Zermelo's objection, which is based on Poincare's recurrence theorem, obviously does not apply as there can be no recurrence theorem for regular density functions ρ. Let us emphasize in this connection that both P_0 and Λ cannot be defined to act on phase points or singular distributions, but must necessarily be defined as only acting on regular density functions.

Loschmidt's objection which is based on symmetry of dynamical evolution under velocity inversion is deeper. Indedd, computer calculation of Boltzmann's H quantity

$$H_B = \int f(v) \log f(v) dv \quad ,$$

where f(v) is the one-particle velocity distribution, has been made for a system of hard disks. If one starts with an initial distribution based on lattice sites and with isotropic velocity distribution, then one finds that H_B does indeed decrease with time t. However, if all velocities are inverted at time t_0, it is found that H_B behaves antithermodynamically (i.e., increases rather than decreases) in the interval $[t_0, 2t_0]$. This clearly demonstrates that Boltzmann's H theorem cannot be valid for all initial density functions. In particular, it cannot be valid both before and after velocity inversion.

In contrast the H function $\Omega(\rho_t)$ is a monotonically decreasing function of t for *all initial* density ρ as long as the system remains isolated. Velocity inversion at time t_0, may cause a discontinuous jump in $\Omega(\rho_t)$ due to entropy (or information) flow from the external apparatus implementing the velocity inversion; but $\Omega(\rho_t)$ again continues to decrease as soon as the operation of velocity inversion is completed and the system is again isolated from the outside. At no stage is there any antithermodynamic behavior. In any cycle in which the system returns to its initial state ρ_0 the net entropy flow dS_e from the outside to the system is negative in agreement with the thermodynamic principle that the entropy production $dS_i = -dS_e$ inside the system is positive. Let us illustrate this explicitly in the case that the initial state is symmetric under velocity inversion $V\rho = \rho$, and one takes $\tilde{\rho}_t = P_0 U_t \rho$ in defining $\Omega(\rho_t)$.

Now, using the notation $\Omega(t) \equiv \Omega(\rho_t)$

$$\Omega(0) = \int (P_0\rho) \ln (P_0\rho) d\mu$$

$$\begin{aligned} \Omega(t_{0-}) &= \int_\Gamma (P_0 U_{t_0}\rho) \ln (P_0 U_{t_0}\rho) d\mu \\ &= \int_\Gamma (U_t^* P_0 U_t \rho) \ln (U_{t_0}^* P_0 U_{t_0} \rho) d\mu \\ &= \int (P_{-t_0}\rho) \ln (P_{-t_0}\rho) d\mu \le \Omega(0) \quad , \quad t_0 \ge 0 \quad . \end{aligned}$$

(Here the first equality follows because the expression $\int \rho \ln \rho \, d\mu$ is invariant under dynamical evolution U_t, and the inequality follows because P_{-t_0} is a coarse graining operation with respect to a coarser partition than that of P_0).

If velocities are inversed at t_0 the H function $\Omega(t_{0+})$ immediately after this operation is given by

$$\begin{aligned} \Omega(t_{0+}) &= \int_\Gamma (P_0 V U_{t_0}\rho) \ln (P_0 V U_{t_0}\rho) d\mu \\ &= \int_\Gamma (P_0 U_{t_0}^* V\rho) \ln (P_0 U_t^* V\rho) d\mu \\ & \int_\Gamma (P_{t_0} V\rho) \ln (P_{t_0} V\rho) d\mu = \int (P_{t_0}\rho) \ln (P_{t_0}\rho) d\mu \quad . \end{aligned}$$