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THE FUNCTIONAL DERIVATIVE AND ITS USE IN THE
DESCRIPTION OF NOISY DYNAMICAL SYSTEMS

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1. INTRODUCTION

In this series of two lectures we present an introduction into the method of the functional derivative and give some useful applications taken from the topic of stochastic flows. This important method enters a variety of fields in science. For example, we are all familiar with its use in mechanics where the method of the functional derivative is utilized in the derivation of the Euler-Lagrange equation. Other important applications can be found within the topics of wave propagation in randomly inhomogeneous media, path integral methods in quantum mechanics and in statistical mechanics, or in many body theory. Here, our main focus, however, will be in methods of solving differential equations containing random functions (noise sources) as they occur, e.g. in the description of

(b) In mechanics, we often consider a functional known as the action

$$\mathcal{L}[x] = \int_{t_1}^t L(x(t), \dot{x}(t), t) dt \quad (4)$$

where L denotes the Lagrange function characterizing the system under consideration.

(c) Another example taken from the statistical mechanics of non-ideal gases is the free energy of a gas in a volume V with an interaction potential, $U(\underline{r}) = U(\underline{r}_1 - \underline{r}_j = \underline{r})$, between two particles. With T the temperature, k the Boltzmann constant and N the total number of particles we have for the free energy per unit volume

$$F[U] = F_{ideal}(T, N/V) - \frac{kT}{V} \int \exp\left\{-\frac{1}{kT} \sum_{i < j} U(\underline{r}_i - \underline{r}_j)\right\} d\mathbf{r}_1 \dots d\mathbf{r}_N \quad (5)$$

(d) Finally, we mention here the characteristic functional of a random process $x(t)$. The characteristic function of n random variables $\{x_1, \dots, x_n\}$ is the expectation

$$\chi(\phi_1, \dots, \phi_n) = \langle \exp i \sum_{m=1}^n \phi_m x_m \rangle \quad (6a)$$

which upon the introduction of a continuous index $m \rightarrow t$, (i.e. $\phi_m \rightarrow \phi(t)$), yields the characteristic functional

$$\chi[\phi] = \langle \exp i \int \phi(t) x(t) dt \rangle ; \chi[\phi=0] = 1. \quad (6b)$$

Also note, that (6a) is recovered from (6b) by considering the function-element

$$\phi(t) = \phi_1 \delta(t-t_1) + \dots + \phi_n \delta(t-t_n) \quad (6c)$$

Often one is not interested in the whole functional, but rather in the element $\bar{x}(t)$ at which the functional becomes extremal or "stationary". In other cases, one is actually only interested in the change of $F[\phi]$ upon a slight change of the element $\phi \rightarrow \phi + \delta\phi$. All of that naturally involves the concept of a "derivative after the

parametric oscillators driven by random forces, the statistical mechanics of coarse grained variables (Mori-type equations) or for the modeling of the statistical properties of observables near threshold to instabilities.¹⁾

2. THE NOTION OF A FUNCTIONAL

Before we go on into more heavy stuff, let us first recall the meaning of a functional. Let us consider a function of several variables $\{\phi_1, \dots, \phi_n\}$

$$F = F(\phi_1, \dots, \phi_i, \dots, \phi_n) \quad (1)$$

If we now look upon the index i as a continuous variable, $i \rightarrow t$, we arrive at a functional $F[\phi]$. Given a function $\hat{\phi}(t)$, a functional

$$F = F[\hat{\phi}] \quad (2)$$

is the prescription which assigns a value for each given "element" $\hat{\phi}(t)$ (see Fig. 1)



Fig. 1: Definition of a Functional

Some familiar examples would be:

(a) The area formed by a real-valued, positive function $\phi(x)$, $a < x < b$, is determined by the functional

$$F[\phi] = \int_a^b \phi(x) dx \quad (3)$$

function element ϕ ; i.e. the functional derivative $\delta F/\delta\phi$. Anticipating some results, which we will belabor below, we have for the examples, (a) - (d), the results:

- (a) $\delta F/\delta\phi(x) = \phi(x)$, the function-value at x .
- (b) $\delta L/\delta\dot{x}(t) = 0$, yielding the Euler-Lagrange equation for the classical path $\bar{x}(t)$.
- (c) $\delta F/\delta U(\underline{x}) = \rho(\underline{x})$, the pair distribution function.
- (d) $-i \delta \chi/\delta \phi(t) \Big|_{\phi=0} = \langle x(t) \rangle$, the mean value of $x(t)$.

Having understood at this point somewhat the purpose of functional derivatives we now present its definition.

3. DEFINITION OF THE FUNCTIONAL DERIVATIVE

3.1. Mathematical Definition

Let A denote an operator (not necessarily linear) acting on a Banach space (i.e. we have a norm $||\dots||$). Then we call the operator A differentiable, if there exists a linear and bounded operator, $\delta A/\delta f$, obeying

$$|| A(f+h) - Af - \frac{\delta A}{\delta f} h || \leq ||h|| \varepsilon \quad ||h|| \quad (7)$$

for all h with $||h||$ less than some small number δ and $\varepsilon(x)$ the "zero-function", i.e. $\varepsilon(x) \rightarrow 0$ with $x \rightarrow 0$. Note also that the linear (and continuous) operator $\delta A/\delta f$ generally depends nonlinear on the element f . The operator $\delta A/\delta f$ is known as the functional derivative, often also named the variation derivative or Fréchet-derivative, since he was the first to introduce this concept.²⁾ Writing the inner product of $\delta A/\delta f$ with h as an (eventually only formal) integral; i.e.

$$\langle \delta A/\delta f | h \rangle = \int \frac{\delta A}{\delta f(t)} h(t) dt \quad (8)$$

gives perfect sense to the notation $\delta A/\delta f(t)$ as being the change of a functional $Af \equiv \phi(f)$ upon a minor change of f at position t .

Example: Let us consider the change ΔL of the action in (4)

$$\begin{aligned} \Delta L &= L[x + \xi] - L[x] \\ \Delta L &= \int_{t_1}^{t_2} \left\{ \frac{\partial L}{\partial x(t)} \xi(t) + \frac{\partial L}{\partial \dot{x}(t)} \dot{\xi}(t) + o(|\xi|^2) \right\} dt \end{aligned}$$

With a partial integration of the 2-nd term we get

$$\begin{aligned} \Delta L &= \int_{t_1}^{t_2} \left\{ \frac{\partial L}{\partial x(t)} - \left(\frac{d}{dt} \frac{\partial L}{\partial \dot{x}(t)} \right) \right\} \xi(t) dt \\ &+ \xi(t) \frac{\partial L}{\partial \dot{x}(t)} \Big|_{t_1}^{t_2} + o(|\xi|^2) \end{aligned}$$

Now we can read of the functional derivative from (8), yielding

$$\frac{\delta L}{\delta x(t)} = \left(\frac{\partial L}{\partial x(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}(t)} \right) + \frac{\partial L}{\partial \dot{x}(t)} [\delta(t-t_2) - \delta(t-t_1)]$$

If we impose zero end-variations on $\xi(t)$, i.e. $\xi(t)=0$ at $t=t_1, t=t_2$ (Lagrange principle), we end up with the well-known Euler-Lagrange equation for the extremal path $\bar{x}(t)$

$$\frac{\delta L}{\delta \bar{x}(t)} = 0 = \left(\frac{\partial L}{\partial \bar{x}(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\bar{x}}(t)} \right)$$

3.2 A Down-to-Earth Definition

We consider the values of the same functional for the functions $\phi(t)$ and $\phi(t) + \delta\phi(t)$, where $\delta\phi(t) \neq 0$ in a small interval, $s-\frac{1}{2}\Delta t \leq t \leq s+\frac{1}{2}\Delta t$, i.e. we vary the functions $\phi(t)$ near the position s , see Fig. 2.

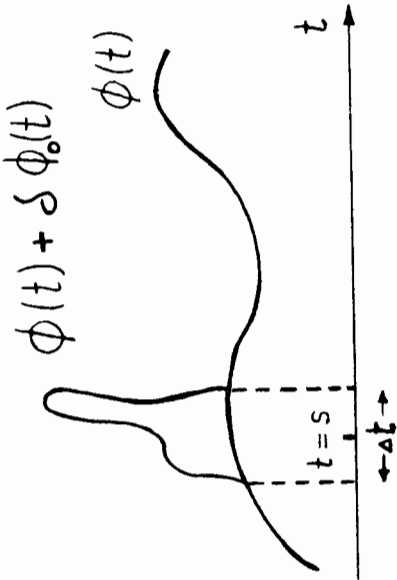


Fig. 2: For the Definition of the Functional Derivative

The functional derivative is then defined as the limit

$$\frac{\delta F[\phi]}{\delta \phi(s)} \equiv \lim_{\Delta t \rightarrow 0} \frac{F[\phi + \delta \phi] - F[\phi]}{\int \delta \phi(t) dt} \Delta t \tag{9}$$

Before we proceed further, let us exercise this limiting procedure with an example of a quadratic functional $F[\phi]$

$$F[\phi] = \iint g(t,s) \phi(t) \phi(s) dt ds$$

Therefore we have

$$F[\phi + \delta \phi] - F[\phi] = \iint g(t,s) [\phi(t)\delta\phi(s) + \phi(s)\delta\phi(t)] dt ds + O(\delta\phi^2)$$

Using for the second part of the integral a substitution of variables, i.e. $t \rightarrow s, s \rightarrow t$, we obtain

$$\Delta F[\phi] = \int \phi(t) dt \int ds \{g(t,s) + g(s,t)\} \delta\phi(s) .$$

We now vary the function ϕ around the position $t = s \equiv \tau$. Next we apply the average theorem for integrals and get $\tau - \frac{1}{2}\Delta t \leq \bar{s} \leq \tau + \frac{1}{2}\Delta t$

$$\delta F[\phi] = \int \phi(t) \{g(t, \bar{s}) + g(\bar{s}, t)\} dt \int \delta \phi(s) ds \Delta t$$

Observing that

$$A \equiv \iint \{g(t,s) - g(s,t)\} dt ds = \iint \{g(s,t) - g(t,s)\} dt ds = -A$$

We can assume without loss of generality that $g(t,s)$ is symmetric in its arguments thereby obtaining for the limit in (9) the result

$$\frac{\delta F[\phi]}{\delta \phi(\tau)} = 2 \int g(t,\tau) \phi(t) dt .$$

4. DOING THE FUNCTIONAL DERIVATIVE

Looking at the above example one might wonder if the result could not have been obtained in much simpler terms, thereby short-cutting the detailed limiting procedure. This is indeed true in most cases. If we remember that the functional can be looked upon as the continuum limit of a multivariable function we might perturb the functional at the position $t=\tau$ by varying the "variable" $\phi_\tau \equiv \phi(\tau)$, by an amount $\delta\phi(\tau) = \lambda\delta(t-\tau)$. Alternatively, we may then express the limit in (9) as the limit of the "directional derivative"

$$\frac{\delta F[\phi]}{\delta \phi(\tau)} = \left. \frac{dF[\phi(t) + \lambda\delta(t-\tau)]}{d\lambda} \right|_{\lambda=0} , \tag{10}$$

assuming that both sides (eventually only in the sense of a distribution) exist. Clearly, this concept is also readily extended to multidimensional functionals $F[\phi(t)] = F[\phi_1(t), \dots, \phi_n(t)]$

$$\frac{\delta F[\phi]}{\delta \phi_i(\tau)} = \left. \frac{dF[\phi_1(t), \dots, \phi_i(t) + \lambda\delta(t-\tau), \dots, \phi_n(t)]}{d\lambda} \right|_{\lambda=0} \tag{11}$$

With this trick, (10), in mind, our job becomes considerably simplified. Exercising this method, we immediately arrive at the following useful relations

$$1. F[\phi] = f(\phi(t))$$

$$\frac{\delta F[\phi]}{\delta \phi(\tau)} = \frac{\partial f}{\partial \phi} \delta(t-\tau) \tag{12}$$

$$2. F[\phi] = f(g(\phi))$$

$$\frac{\delta F[\phi]}{\delta \phi(\tau)} = \frac{\partial f}{\partial g} \frac{\delta g}{\delta \phi(\tau)} \tag{13}$$

thereby defining the cumulants, $C_n(t_1, \dots, t_n)$ as

$$C_n(t_1, \dots, t_n) = \frac{1}{i^n} \frac{\delta^n \psi[\phi]}{\delta \phi(t_1) \dots \delta \phi(t_n)} \Big|_{\phi=0} \quad (20)$$

6. IMPORTANT CORRELATION FORMULAE

By now we have warmed up enough to actually apply the technique of functional derivatives to more interesting situations. As a first major application we consider the correlation of a functional $g\{x(t); t_0 \leq t \leq t_f\}$ of a stochastic process $x(t)$, defined on the observation interval $t \in [t_0, t_f]$, with the stochastic process $x(t)$ itself; i.e.

$$\langle x(t) g[x] \rangle, \quad t < t_f \quad (21)$$

Our principal goal is to disentangle the correlation in (21) into its most transparent form in terms of the intrinsic properties of the stochastic process, such as its cumulant properties. For reasons which will become clear very soon we complicate the situation by introducing an auxiliary, deterministic function $\eta(t)$ into the correlation (21); i.e. following Reference 3, we consider the expression $\langle x(t) g[x+\eta] \rangle$. Upon expanding $g[x+\eta]$ in x , see (18), we generate the moments of $x(t)$

$$\begin{aligned} \langle x(t) g[x+\eta] \rangle &= \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int dt_1 \dots dt_n \frac{\delta^n g[\eta]}{\delta \eta(t_1) \dots \delta \eta(t_n)} \\ &\quad \cdot \langle x(t_1) x(t_2) \dots x(t_n) x(t) \rangle \end{aligned}$$

In terms of the property in (19), this can be recast as

$$\begin{aligned} &= \sum_{n=0}^{\infty} \frac{1}{n!} \frac{1}{(i)^{n+1}} \int \dots \int dt_1 \dots dt_n \frac{\delta^n g[\eta]}{\delta \eta(t_1) \dots \delta \eta(t_n)} \\ &\quad \cdot \frac{\delta^n}{\delta \phi(t_1) \dots \delta \phi(t_n)} \left(\frac{\delta \chi[\phi]}{\delta \phi(t)} \right) \Big|_{\phi=0} \end{aligned}$$

Note that the term $(\delta \chi / \delta \phi)$ can be written as $(\chi \delta \ln \chi / \delta \phi)$. With $\ln \chi = \psi$, we can utilize the Leibnitz rule for the functional product

$$3. \quad \begin{aligned} F[\phi] &= f(\phi(t), \dot{\phi}(t)) \\ \frac{\delta F[\phi]}{\delta \phi(t)} &= \frac{\partial f}{\partial \phi} \delta(t-\tau) - \frac{\partial f}{\partial \dot{\phi}} \frac{d}{dt} \delta(t-\tau) \end{aligned} \quad (14)$$

$$4. \quad \begin{aligned} F[\phi] &= \int f(\phi, \dot{\phi}) dt \\ \frac{\delta F[\phi]}{\delta \phi(\tau)} &= \frac{\partial f}{\partial \phi(\tau)} - \frac{d}{dt} \frac{\partial f}{\partial \dot{\phi}(\tau)} \end{aligned} \quad (15)$$

5. HIGHER ORDER FUNCTIONAL DERIVATIVES

The functional derivative $\delta A / \delta f$ is a linear operator which generally depends nonlinear on the element f . Thus, the mapping $\delta A / \delta f$, h held fixed, can be differentiated as before, (7); i.e. with

$$\begin{aligned} \frac{\delta}{\delta f} \left(\frac{\delta A}{\delta f} h \right) g &\equiv \frac{\delta^2 A}{\delta f^2} h g \\ \left| \left| \frac{\delta A}{\delta f} h \right|_{f+g} - \frac{\delta A}{\delta f} h \right| &\leq \|g\| \varepsilon(\|g\|) \end{aligned} \quad (16)$$

This procedure can be continued to give the functional Taylor series

$$A(f+h) = Af + \frac{\delta A}{\delta f} h + \frac{1}{2!} \frac{\delta^2 A}{\delta f^2} h h + \dots + \frac{1}{n!} \frac{\delta^n A}{\delta f^n} h \dots h + \dots \quad (17)$$

For example, the functional $A(x+\eta) = g[x+\eta]$ is expanded in $x(t)$ as

$$\begin{aligned} g[x + \eta] &= g[\eta] + \int dt_1 \frac{\delta g[\eta]}{\delta \eta(t_1)} x(t_1) + \dots \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \int \dots \int dt_1 \dots dt_n \frac{\delta^n g[\eta]}{\delta \eta(t_1) \dots \delta \eta(t_n)} x(t_1) \dots x(t_n) \end{aligned} \quad (18)$$

Examples: From (6b), the n -th order functional derivative immediately yields the n -th order moment m_n

$$i^{-n} \frac{\delta^n \chi[\phi]}{\delta \phi(t_1) \dots \delta \phi(t_n)} \Big|_{\phi=0} = \langle x(t_1) x(t_2) \dots x(t_n) \rangle = m_n(t_1, \dots, t_n) \quad (19)$$

The cumulant generating functional $\psi[\phi]$ is given by

$$\psi[\phi] = \ln \chi[\phi]$$

differentiation

$$\frac{\delta^n}{\delta \phi^n} (X \frac{\delta \psi}{\delta \phi}) = \sum_{m=0}^n \binom{n}{m} \frac{\delta^{n-m}}{\delta \phi^{n-m}} X \frac{\delta^m}{\delta \phi^m} \left(\frac{\delta \psi}{\delta \phi} \right)$$

Note that the functional derivatives of the second term generates a (m+1)-order cumulant if evaluated at $\phi=0$, (see (20)). Therefore, by use of the notation in (19), (20), we arrive at

$$\langle x(t) g[x+\eta] \rangle = \sum_{n=0}^{\infty} \sum_{m=0}^n \frac{1}{m!(n-m)!} \int \dots \int dt_1 \dots dt_n \cdot C_{m+1}(t, t_1, \dots, t_m, t_{m+1}, \dots, t_n) \cdot \frac{\delta^n g[\eta]}{\delta \eta(t_1) \dots \delta \eta(t_n)}$$

In the next step, we reverse the order of the sums. This yields with $k=n-m$

$$\begin{aligned} &= \sum_{m=0}^{\infty} \frac{1}{m!} \int \dots \int dt_1 \dots dt_m C_{m+1}(t, t_1, \dots, t_m) \\ &\cdot \frac{\delta^m}{\delta \eta(t_1) \dots \delta \eta(t_m)} \sum_{k=0}^{\infty} \frac{1}{k!} \int \dots \int dt_1 \dots dt_k \\ &\cdot m_k(t_1, \dots, t_k) \frac{\delta^k g[\eta]}{\delta \eta(t_1) \dots \delta \eta(t_k)} \end{aligned}$$

The second sum, however, simply sums up to $\langle g[x+\eta] \rangle$, see (18); i.e.

$$\begin{aligned} \langle x(t) g[x+\eta] \rangle &= \sum_{m=0}^{\infty} \frac{1}{m!} \int \dots \int dt_1 \dots dt_m C_{m+1}(t, t_1, \dots, t_m) \\ &\cdot \frac{\delta^m}{\delta \eta(t_1) \dots \delta \eta(t_m)} \langle g[x+\eta] \rangle \end{aligned}$$

At this point, we now set $\eta(t) = 0$. Thus we obtain the central result 3-5)

$$\begin{aligned} \langle x(t) g[x] \rangle &= \sum_{n=0}^{\infty} \frac{1}{n!} \int_{t_0}^{t_f} \dots \int_{t_0}^{t_f} dt_1 \dots dt_n C_{n+1}(t, t_1, \dots, t_n) \\ &\cdot \left\langle \frac{\delta^n g[x]}{\delta x(t_1) \dots \delta x(t_n)} \right\rangle \end{aligned} \tag{22}$$

Taking two arbitrary processes, $\{x(t), y(s)\}$, with cumulants $C_{n,m}^{x,y}(t_1, \dots, t_n; s_1, \dots, s_m)$, the above exercise can be repeated to obtain for the correlation of two functionals $f[x]$ and $g[y]$ the non-trivial result.

$$\begin{aligned} \langle f[x] g[y] \rangle &= \langle f[x] \rangle \langle g[y] \rangle \\ &+ \sum_{n=1}^{\infty} \frac{1}{n!} \prod_{i=1}^n \sum_{m_i, k_i=1}^{\infty} \frac{1}{m_i! k_i!} \int \dots \int dt_1^{(i)} \dots dt_{m_i+k_i}^{(i)} \dots ds_{k_i}^{(i)} \\ &\cdot C_{m_i, y}^{x, y}(t_1^{(i)}, \dots, t_{m_i}^{(i)}; s_1^{(i)}, \dots, s_{k_i}^{(i)}) \left\langle \frac{\delta^{m_1+\dots+m_n} f[x]}{\delta x(t_1^{(1)}) \dots \delta x(t_{m_n}^{(n)})} \right\rangle \\ &\cdot \left\langle \frac{\delta^{k_1+\dots+k_n} g[y]}{\delta y(s_1^{(1)}) \dots \delta y(s_{k_n}^{(n)})} \right\rangle \end{aligned} \tag{23}$$

Problem 1: By use of the relation given in Ref. 5 ,

$$\begin{aligned} \frac{\delta^n \langle f[x] g[y] \rangle}{\delta C_{p_1, q_1}^{x, y} \dots \delta C_{p_n, q_n}^{x, y}} &= \left\langle \frac{\delta^{p_1+\dots+p_n} f[x]}{\delta x(t_1^{(1)}) \dots \delta x(t_{p_n}^{(n)})} \frac{\delta^{q_1+\dots+q_n} g[y]}{\delta y(s_1^{(1)}) \dots \delta y(s_{q_n}^{(n)})} \right\rangle \\ &\cdot \prod_{i=1}^n \frac{1}{p_i! q_i!} \end{aligned} \tag{24}$$

derive the result in (23), upon expanding first $\langle f[x] g[y] \rangle$ into a functional Taylor series in the cumulants $C_{p_i, q_i}^{x, y}$.

Problem 2: Consider the case that the set $\{x(t), y(s)\}$ are Gaussian processes. In other words, all cumulants $C_{p,q}^{x,y} = 0$ for $p + q > 2$.

Show that (23) simplifies to the useful result⁵⁾

$$\begin{aligned} \langle f[x]g[y] \rangle &= \langle f[x] \rangle \langle g[y] \rangle \\ &+ \sum_{n=1}^{\infty} \frac{1}{n!} \int_{t_0}^t \dots \int_{t_0}^t \frac{\delta^n f[x]}{\delta x(t_1) \dots \delta x(t_n)} \langle \dots \rangle \\ &\cdot \langle \frac{\delta^n g[y]}{\delta y(s_1) \dots \delta y(s_n)} \rangle \prod_{i=1}^n C_{1,1}^{x,y}(t_i, s_i) dt_i ds_i \end{aligned} \quad (25)$$

In particular, for $f[x] = x(t)$, $y(t) = g(x(t))$, one obtains the Furutsu-Novikov result⁹⁾

$$\langle x(t)g[x] \rangle = \langle x(t) \rangle \langle g[x] \rangle + \int_{t_0}^t C_2(t, s) \langle \frac{\delta g[x]}{\delta x(s)} \rangle ds \quad (26)$$

which also equals the result in (22) after the 2nd term, because $C_n = 0$ for $n > 2$ for a Gaussian process and $C_1(t) = \langle x(t) \rangle$.

Problem 3: Setting $g[x]$ in (22) equal to a polynomial, i.e.

$$g[x] = x(t_1) x(t_2) \dots x(t_{n-1})$$

derive the resulting recursive relationship between moments and cumulants.³⁾

In particular, if $x(t) = x$ is a random variable, show that this relationship reduces for $n > 1$ to

$$C_n = \langle x^n \rangle - \sum_{m=1}^{n-1} \binom{n-1}{m-1} C_m \langle x^{n-m} \rangle, \quad n > 1 \quad (27)$$

where C_n denotes the n -th order cumulant of x .

The useful correlation formulae (22), (23), (25) (26) are valid if the latest time t occurring in the functional $f[x]$, e.g. $f[x] = x(t)$, is less than the final observation t_f , i.e. $t < t_f$.

Actually, the above formulas remain true also for $t \leq t_f$ if the cumulants of the driving process are not white (i.e. not δ -correlated in time).³⁾ The case of δ -correlated random processes requires some special care if times up to $t = t_f$ are considered. In that case, it is advantageous to focus on the curtailed cumulant generating functional ψ_t

$$\psi_t[v] = \ln X_t[v] = \ln \langle \exp i \int_{t_0}^t ds v(s)x(s) \rangle \quad (28)$$

Then, by use of the auxiliary functional $\Sigma_t[v]$

$$\Sigma_t[v] = \frac{-i}{v(t)} \frac{\partial}{\partial t} \psi_t[v] \quad (29)$$

we obtain with δ -correlated processes for (22)⁶⁾

$$\langle x(t_f) g[x] \rangle = \langle \Sigma_{t_f} \left[\frac{\delta}{i \delta x(t_f)} \right] g[x] \rangle \quad (30)$$

7. AN INTEGRAL EQUATION FOR THE FUNCTIONAL DERIVATIVE

Throughout the rest of this lecture we are interested in the solution of differential equations containing random forces. The archetype of such random flows can be cast into the form of a nonlinear Langevin equation. For the sake of clarity only, we again restrict the discussion to a one-dimensional process $x(t)$ driven by a random noise $\xi(t)$. If we also allow for a multiplicative noise coupling with a coupling function $g(x(t))$ we arrive at the stochastic differential equation

$$\dot{x} = A(x) + g(x) \xi(t) \quad (31)$$

For a variety of many applications of such types of equations we refer the reader to Ref. 1 and to the other articles in this book. The formal integral of (31) now reads

$$x(t) = \int_{t_0}^t \{A(x(s)) + g(x(s)) \xi(s)\} ds + x(t_0) \quad (32)$$

Using repeatedly the chain rule (12) and (13) (e.g. $\delta \xi(s) / \delta \xi(t) = \delta(s-t)$) we obtain for the functional derivative

$$\frac{\delta x(t)}{\delta \xi(\tau)} = \int_{\tau}^t \left\{ \frac{\partial A}{\partial x(s)} \frac{\delta x(s)}{\delta \xi(\tau)} + \delta(s-\tau) g(x(s)) \right. \\ \left. + \left(\frac{\partial g}{\partial x(s)} \frac{\delta x(s)}{\delta \xi(\tau)} \right) \xi(s) \right\} ds \quad (33)$$

The lower integration limit is once more due to causality; i.e. the left hand side cannot explicitly depend on times earlier than τ and not on times later than t . Observing (31), we obtain the integro equation⁷⁾ (θ denotes the step function)

$$\frac{\delta x(t)}{\delta \xi(\tau)} = \theta(t-\tau) \{ g(x(\tau)) + \int_{\tau}^t ds \frac{\partial \dot{x}(s)}{\partial x(s)} \frac{\delta x(s)}{\delta \xi(\tau)} \} \quad (34)$$

This relation is quite useful in the study of correlations of the type in (22), which intrinsically contains, by repeated use of the chain rule, the functional derivative. For example, the mean value of (31) reads

$$\langle \dot{x} \rangle = \langle A(x(t)) \rangle + \langle \xi(t) g(x(t)) \rangle \quad (35)$$

where the second term can be disentangled in terms of the cumulants of the noise source $\xi(t)$, (see (22), (30)), yielding fluctuation induced drift terms. For the statistical flows given below, we now exercise the evaluation of the functional derivative in (34).

Example 1: Consider the linear flow

$$\dot{x} = a(t) x(t) + \xi(t) \quad (36)$$

Upon integration, i.e.

$$x(t) = \int_{t_0}^t \chi(t,s) \xi(s) ds + x_0 \chi(t,t_0)$$

where

$$\chi(t,s) = \exp \int_s^t a(\tau) d\tau$$

we readily obtain for the functional derivative from (15) the explicit result

$$\frac{\delta x(t)}{\delta \xi(\tau)} = \theta(t-\tau) \chi(t,\tau) \quad (37)$$

Example 2: Let the stochastic flow be drift-free; i.e.

$$\dot{x} = a(t) g(x(t)) \xi(t) \quad (38)$$

By use of the concept of a random time u ⁸⁾

$$u = \int_{\tau}^t a(s) \xi(s) ds$$

Eq. (38) for $x \{u\} = x(t)$ can be recast as

$$\frac{dx}{du} = g(x(u))$$

At this point we can use the prescription in (10) to obtain the closed result⁸⁾

$$\frac{\delta x(t)}{\delta \xi(\tau)} = \frac{d}{d\lambda} \left\{ x \left(\int_{\tau}^t ds a(s) [\xi(s) + \lambda \delta(s-\tau)] \right) \right\} \Big|_{\lambda=0} \\ = \frac{\partial x}{\partial u} \frac{du}{d\lambda} \Big|_{\lambda=0} \\ = \theta(t-\tau) g(x(t)) a(\tau) \quad (39)$$

where the dependence on the noise enters only via the process $x(t)$ at the final "Markovian" time point t .

Generally, it will not be possible to obtain closed answers for the functional derivative $\delta x(t)/\delta \xi(\tau)$ taken at different times $\tau \neq t$. In evaluating correlation functionals of the type in (22) with $x(t) \equiv \xi(t)$ we are then stuck with the evaluation of averages which depend generally nonlinear on the macroscopic process $x(t)$, as given by (32). For example, in (35), the average of the drift, $\langle A(x(t)) \rangle$, is most conveniently evaluated via the single-event probability $P_t(x)$, i.e.

$$\langle A(x(t)) \rangle = \int P_t(x) A(x) dx$$

However, this requires an equation of motion for the quantity $P_t(x)$.

$$P_t(x) = \langle \delta(x(t)-x) \rangle \\ = \int P_t(x(t)) \delta(x(t)-x) dx(t) \quad (40)$$

Thus, what the doctor orders here, is a derivation of the master equation for (generally non-Markovian) flows of the type in (31) together with its solution - at least within some reasonable approximation. -

8. MASTER EQUATION FOR COLORED NOISE

Going back to (31), we assume that the correlation $\langle \xi(t) \xi(s) \rangle$ has a finite lifetime (colored noise). The rate of change of $p_t(x)$, (40), i.e., the master equation, is then evaluated as

$$\dot{p}_t(x) = \frac{\partial}{\partial t} p_t(x) = - \frac{\partial}{\partial x} \langle \delta(x(t)-x) \dot{x}(t) \rangle \quad (41)$$

If we insert the flow in (31) we obtain

$$\dot{p}_t(x) = - \frac{\partial}{\partial x} (A(x) p_t(x)) - \frac{\partial}{\partial x} g(x) \langle \xi(t) \delta(x(t)-x) \rangle \quad (42)$$

It is here, where we finally can use for the 2nd term the result in (22) to its fullest power. Denoting the cumulants of the process $\xi(t)$ by $C_n(t_1, \dots, t_n)$ we get³⁾

$$\begin{aligned} \dot{p}_t(x) = & - \frac{\partial}{\partial x} (A(x) p_t(x)) - \langle \xi(t) \rangle \frac{\partial}{\partial x} (g(x) p_t(x)) \\ & - \frac{\partial}{\partial x} g(x) \sum_{n=1}^{\infty} \frac{1}{n!} \int_{t_0}^t \dots \int_{t_0}^t dt_1 \dots dt_n \cdot \\ & \cdot C_{n+1}(t, t_1, \dots, t_n) \langle \frac{\delta^n}{\delta \xi(t_1) \dots \delta \xi(t_n)} \delta(x(t)-x) \rangle \end{aligned} \quad (43)$$

The last term can in principle be written out more explicitly by observing the chain rule

$$\frac{\delta}{\delta \xi(\tau)} \delta(x(t)-x) = - \frac{\partial}{\partial x} \delta(x(t)-x) \frac{\delta x(t)}{\delta \xi(\tau)} \quad (44)$$

In the following, we always assume that the noise has zero average

$$C_1(t) = \langle \xi(t) \rangle = 0,$$

thereby canceling the 2nd term in (43). For a Gaussian noise, i.e. $C_n = 0$ for $n > 2$, our eq. (43) simplifies considerably, giving

$$\begin{aligned} \dot{p}_t(x) = & - \frac{\partial}{\partial x} (A(x) p_t(x)) \\ & + \frac{\partial}{\partial x} g(x) \frac{\partial}{\partial x} \int_{t_0}^t ds C_2(t,s) \langle \delta(x(t)-x) \frac{\delta x(t)}{\delta \xi(s)} \rangle \end{aligned} \quad (45)$$

It is at this stage, where we meet serious trouble. If the functional derivative depends upon the process $x(s)$, $t_0 \leq s \leq t$, solely on the "Markovian" end-point $s=t$ we should be very happy, because (43) or (45) yields then a closed equation for $\dot{p}_t(x)$. In most cases of interest, however, we are left with (34), which induces correlations between functionals of the integral in (32), i.e. $\{x(s)\}$, $s \leq t$. This brings us back to the complicated (yet still powerful) relation (23). It is here, where the problem of a reasonable approximation, reflecting the structure in (23), enters the scene. At present time, not much about a general approximation scheme is known. The author is convinced, that each type of nonlinearity and noise structure needs individual, special attention. For noise with a short correlation time, an obvious approximation scheme would consist in expanding the functional derivative, (34), in time around the Markovian time point $\tau=t$. However, such an expansion is not systematic and generally does not converge uniformly.¹⁰⁾ As a matter of fact, if the global behavior of the solution $p_t(x)$ matters for the solution of a problem, wrong results occur likely be use of an approximation truncated at a (2-nd order) Fokker-Planck structure.¹⁰⁾ The cases for which (43) yields a closed equation for the (non-Markovian) single-event probability are certainly not generic. Two such exceptions are given by the flows in (36) and (38). Assuming for the sake of simple elucidation that the noise is Gaussian with zero mean, we obtain from (45) for the master equation of the linear flow (36)³⁾

$$\dot{p}_t(x) = - a(t) \frac{\partial}{\partial x} (x p_t(x)) + \left\{ \int_{t_0}^t ds C_2(t,s) \chi(t,s) \right\} \frac{\partial^2}{\partial x^2} p_t(x) \quad (46)$$

$$\dot{Y}(t-s) = \hat{Y}(t-s) + 2\Omega \delta(t-s)$$

the structure in (48) simplifies to

$$\dot{x} = - \int_0^t \dot{Y}(t-s) x(s) ds + \xi(t) \tag{48b}$$

With $\chi(t)$ obeying (solution via Laplace transform technique)

$$\dot{\chi}(t) = - \int_0^t \dot{Y}(t-s) \chi(s) ds ; \chi(0) = 1 \tag{49}$$

the solution of (48) reads

$$x(t) = X(t) x_0 + \int_0^t X(t-u) \xi(u) du . \tag{50}$$

This yields for the functional derivative the simple exact result

$$\frac{\delta x(t)}{\delta \xi(\tau)} = \theta(t-\tau) X(t-\tau) . \tag{51}$$

The result in (51) implies that the master equation for the flows (48) can be solved for in closed form for an arbitrary statistics of $\xi(t)$ ¹⁴⁾! For example, if $\xi(t)$ is assumed to be Gaussian with zero mean, we obtain from (41)

$$\begin{aligned} \dot{P}_t(x) = & - \frac{\partial}{\partial x} \langle \xi(t) \delta(x(t)-x) \rangle \\ & + \frac{\partial}{\partial x} \left\{ \int_0^t \dot{Y}(t-s) \langle x(s) \delta(x(t)-x) \rangle ds \right\} . \end{aligned}$$

Utilizing (26) for the first term and (25) for the 2nd term, and observing that $\langle x(s) \rangle = X(s) \langle x(0) \rangle$, see (50), we arrive at an exact equation

$$\begin{aligned} \dot{P}_t(x) = & \left\{ \int_0^t ds C_2(t,s) X(t-s) \right\} \frac{\partial^2}{\partial x^2} P_t(x) \\ & + \langle x(0) \rangle \left\{ \int_0^t \dot{Y}(t-s) X(s) ds \right\} \frac{\partial}{\partial x} P_t(x) \end{aligned}$$

In case of the drift-free flow (38), we arrive at⁸⁾

$$\dot{P}_t(x) = \left\{ a(t) \int_0^t ds C_2(t,s) a(s) ds \right\} \left(\frac{\partial}{\partial x} g(x) \right)^2 P_t(x) . \tag{47a}$$

Note the typical non-Markovian features of the master equations in (43, 45, 46, 47a), which consist in a dependence on the initial time $t=0$, and effective diffusion coefficients which possibly take on negative values, depending on the behavior of $C_2(t,s)$. An illustrative case is provided by (47a). Note that $\dot{P}_t(x) = 0$ in (47a) as $t \rightarrow t_0^+$. Moreover, using the new time scale

$$\tau = \int_0^t ds a(s) \int_0^s C_2(s,r) a(r) dr$$

(47a) becomes

$$\dot{P}_\tau(x) = \left(\frac{\partial}{\partial x} g(x) \right)^2 P_\tau(x) . \tag{47b}$$

where all non-Markovian features are scaled away. Nevertheless, the process $x(\tau)$ is still non-Markovian. Its single-event evolution just happens to coincide on the time scale, $t \rightarrow \tau$, with the single-event evolution of a time-homogeneous Markov process with the Fokker-Planck operator (47b).

9. MASTER EQUATION FOR THE MORI-TYPE LANGEVIN EQUATION

By use of projector operator methods, Mori¹¹⁾ succeeded in deriving for a general nonlinear flow a generalized, linear Langevin equation which with $t_0 = 0$ has the form

$$\dot{x} = - \Omega x - \int_0^t \hat{Y}(t-s) x(s) ds + \xi(t) . \tag{48a}$$

Clearly, all the nonlinearities, together with the dependence on initial conditions, are hidden in the memory function and the statistical properties of the generally non-Gaussian random force $\xi(t)$.^{12,13)} Setting

vanishing mean and 2-nd cumulant.

$$C_2(t,s) = \delta(t-s)$$

Following standard mathematical calculus (i.e. we obtain the Stratonovich interpretation for the resulting master equation^{3,15}) we then readily obtain from (45) the (Stratonovich) Fokker-Planck equation

$$\dot{p}_t(x) = - \frac{\partial}{\partial x} (A(x) p_t(x)) + \frac{1}{2} \frac{\partial}{\partial x} g(x) \cdot \frac{\partial}{\partial x} g(x) \cdot p_t(x) \quad (54)$$

Thereby, we utilized (34) for the time point $\tau = t$; i.e.

$$\frac{\delta x(t)}{\delta \xi(t)} = g(x(t)) \quad (55)$$

$$t \text{ and } \int \delta(t-s) ds = \frac{1}{2}.$$

A more fascinating case is the one with white shot-noise $\xi(t)$ ^{3,15}

$$\xi(t) = \sum_{i=1}^{n(t)} z_i \delta(t-t_i); P(n(t)=m) \frac{(\lambda t)^m}{m!} \exp-\lambda t \quad (56)$$

where $n(t)$ is a Poisson process with parameter λ , $\{t_i\}$ are the Poisson arrival times and $\{z_i\}$ is a set of independent random variables with a common probability $\rho(z)$. If $\langle z \rangle = 0$, $\xi(t)$ is of vanishing mean and its cumulants are given by¹⁵

$$C_n(t_1, \dots, t_n) = \lambda \langle z^n \rangle \delta(t_1-t_2) \dots \delta(t_{n-1}-t_n), n > 1 \quad (57)$$

If this noise is substituted into the nonlinear flow (31), we obtain from (30), (see Ref. 3, eq. (3.29) and Appendix) or from (43) with $t_f = t$, upon noting that the proper limit to white shot noise is given by

$$\frac{1}{n!} \int \dots \int dt_1 \dots dt_n C_{n+1}(t, t_1, \dots, t_n) \rightarrow \frac{1}{(n+1)!} \lambda \langle z^{n+1} \rangle, \quad (58)$$

for the master equation the explicit result

$$\dot{p}_t(x) = - \frac{\partial}{\partial x} (A(x) p_t(x)) + \lambda \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} \langle z^n \rangle \frac{\partial^n}{\partial x^n} g(x) p_t(x) \quad (59a)$$

$$- \left\{ \int_0^t \gamma(t-s) \int_0^s dr_1 \int_0^{r_1} dr_2 \chi(s-r_1) \chi(t-r_2) C_2(r_1, r_2) \right\} \quad (52)$$

$$\cdot \frac{\partial^2}{\partial x^2} p_t(x)$$

Note that (52) involves an explicit dependence on the initial probability via the initial average ("nonlinear" master equation). Furthermore, if the Green's function $\chi(t)$, (49), takes on no negative values, including zero, (48) can be recast into a time-convolution-less form

$$\dot{x}(t) = \left(\frac{d}{dt} \ln \chi(t) \right) x(t) + \chi(t) \frac{d}{dt} \int_0^t \frac{\chi(t-s)}{\chi(t)} \xi(s) ds, \quad (53)$$

which can be used to derive a "linear", exact master equation; i.e. one which is closed and does not depend on the initial probability $P_0(x)$ ^{3,14}

10. THE WHITE NOISE CASE

The limiting case of white noise is beset with some danger as already mentioned earlier. This has its origin in the fact that the integrals of the type encountered in (32) are not uniquely defined, due to the unbounded variation of the corresponding sample paths. This led to the sujet of Ito versus Stratonovich calculus which gave rise to much, but probably unnecessary, discussion in recent years. (Those debates were mostly limited to the case of white Gaussian noise.) The situation for Master equations, where the elementary driving noise is generalized White Poisson noise, has been discussed by the author in Refs. 3, 15 and 16. A somewhat unwary scientist is being referred to those papers and we hope that any previous confusion will be dissipated rapidly.

Despite those subtleties inherent to white noise, its overwhelming advantage lies in the fact that functional derivatives in formulae of the type in (22-26) need only be evaluated at the latest time point, due to the δ -correlated nature of the corresponding cumulants. Let us consider first the case of white Gaussian noise of

This can be recast as³⁾

$$\dot{p}_t(x) = -\frac{\partial}{\partial x} (A(x) p_t(x)) + \lambda \int dz \rho(z) \{-1 + \exp[-z \frac{\partial}{\partial x} g(x)]\} p_t(x) \quad (59b)$$

If (59) is put into a Kramers-Moyal form;³⁾ i.e. into the form

$$\dot{p}_t(x) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \left(\frac{\partial}{\partial x}\right)^n (A_n(x) p_t(x))$$

we readily observe that each Kramers-Moyal moment $A_n(x)$ contains fluctuation-induced contributions from all higher order moments A_i , $i > n$.^{3,15b)}

Problem Consider the flow in (31) with white shot noise of vanishing mean; i.e.

$$\xi(t) = \sum_{i=1}^n z_i \delta(t-t_i) - \lambda/a$$

and an exponential probability for the random variable z_i

$$\rho(z) = a \exp -az ; a > 0, z > 0, \langle z \rangle = 1/a .$$

Show that the stationary probability $\bar{p}(x)$ of the corresponding master equation equals¹⁷⁾

$$\bar{p}(x) = N^{-1} \frac{|g(x)|}{D(x)} \left[\exp \int^x \frac{A(y) dy}{D(y)} \right] \theta(D(x)) \quad (60)$$

where $D(x) = \frac{\lambda}{a} g(x) [g(x) - A(x)a/\lambda]$, N the normalization, and θ

denotes the step function expressing the support of $\bar{p}(x)$.

11. FORMULAE FOR TELEGRAPHIC NOISE

For the sake of completeness, we review in this last chapter some useful results of Klyatskin's paper¹⁸⁾ on telegraphic noise, also known as dichotomic noise. Telegraphic noise $\xi(t)$, see Fig. 3, is defined by the expression

$$\xi(t) = a(-1)^{n(t)}$$

where $n(t) \equiv n(0,t)$ is a Poisson process with parameter λ .

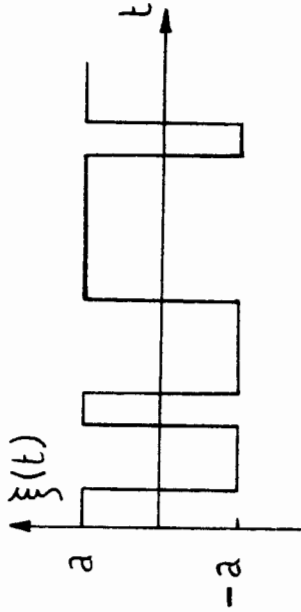


Fig. 3: Realization of the Telegraphic Noise

In other words, $\xi(t)$ is a two-state Markov process. It often serves as the model noise source in colored noise phenomena, e.g. in the study of memory effects in noise induced transitions,¹⁹⁾ and recently in the study of memory effects on escape rates of nonlinear, bistable flows.^{17b,20)} Its statistical properties are readily evaluated. For example, the mean is given by

$$\langle \xi(t) \rangle = a \sum_{m=0}^{\infty} (-1)^m P(n(t)=m)$$

$$= a \exp -\lambda t \sum_{m=0}^{\infty} \frac{(-1)^m (\lambda t)^m}{m!}$$

$$= a \exp -2\lambda t, \quad t > 0$$

The correlation is

$$(61)$$

$$\langle \xi(t) \xi(s) \rangle = a^2 \langle (-1)^{n(0,t) + n(0,s)} \rangle, \quad t > s$$

$$= a^2 \langle (-1)^{2n(0,s) + n(s,t)} \rangle$$

$$= a^2 \langle (-1)^{n(s,t)} \rangle = a^2 \exp -2\lambda |t-s| \quad (62)$$

In particular, note that the correlation is time-homogeneous despite the fact that $\xi(t)$ is not stationary. By use of the initial probability for the step

$$\rho(a) = \frac{1}{2} \{ \delta(a+a_0) + \delta(a-a_0) \},$$

$\xi(t)$ assumes zero mean. For the sequence of time points $\{t_1 \geq t_2 \geq \dots \geq t_n\}$ we then obtain

$$\langle \xi(t_1) \dots \xi(t_n) \rangle = \langle \xi(t_1) \xi(t_2) \dots \xi(t_n) \rangle, \text{ i.e.} \quad (63)$$

$$m_n = a_0^2 \exp - 2\lambda(t_1 - t_2)^{m_{n-2}},$$

because the statistics in the non-overlapping regions (t_1, t_2) and (t_3, t_n) are independent of each other. The result in (63) can be generalized to give with $t_1 \geq t_2 \geq \tau$ for the correlation with a functional $g[\xi(\tau)]$:

$$\langle \xi(t_1) \xi(t_2) g[\xi(\tau)] \rangle = \langle \xi(t_1) \xi(t_2) \rangle \langle g[\xi(\tau)] \rangle \quad (64)$$

The analogue of the correlation formula in (22), where the functional $g_t[\xi]$ is composed of telegraphic noise $\xi(\tau)$, $0 < \tau \leq t$, has been derived first in Ref. (18).

$$\langle \xi(t) g_t[\xi] \rangle = a_0^2 \int_0^t ds \exp - 2\lambda(t-s) \cdot \frac{\delta}{\delta \xi(s)} g_t[\xi(\tau)\theta(s-\tau)] \rangle \quad (65)$$

where the noise-dependence in $g_t[\xi]$ is switched off for times

$$\tau > s, \text{ i.e. } \xi(\tau) \equiv 0, \tau > s.$$

If this telegraphic noise is substituted into the nonlinear flow (31) we obtain from (42) by use of (65)

$$\dot{p}_t(x) = - \frac{\partial}{\partial x} (A(x)p_t(x)) - \frac{\partial}{\partial x} g(x) a_0^2 \int_0^t ds \exp - 2\lambda(t-s) \frac{\delta}{\delta \xi(s)} \tilde{\delta}_t(x(t)-x) \rangle \quad (66)$$

where $\tilde{\delta}_t = \delta_t[\xi(\tau) \theta(s-\tau)]$. From the dynamical equation we have, with $\delta_t \equiv \delta(x(t)-x)$ satisfying

$$\dot{\delta}_t = - \frac{\partial}{\partial x} (A(x)\delta_t) - \frac{\partial}{\partial x} (g(x))\xi(t)\delta_t,$$

and $\delta_{t=s} = \delta(x(s)-x)$, for $\tau > s$; i.e. $\xi(\tau)$ is being switched off, for $\tilde{\delta}_t$ the differential equation

$$\frac{d}{dt} \tilde{\delta}_t = (- \frac{\partial}{\partial x} A(x))\tilde{\delta}_t, \quad \tau > s \quad (67)$$

It has the solution

$$\tilde{\delta}_t = \delta(x(s)-x) \exp \left\{ - \frac{\partial}{\partial x} A(x)(t-s) \right\} \quad (68)$$

Now, the functional derivative in (66) can readily be performed

$$\frac{\delta}{\delta \xi(s)} (\delta_{t=s}) = - \frac{\partial}{\partial x} g(x) \delta(x(s)-x)$$

Thus, we end up with an exact, retarded non-Markovian Master equation

$$\dot{p}_t(x) = - \frac{\partial}{\partial x} (A(x)p_t(x)) + a_0^2 \frac{\partial}{\partial x} g(x) \int_0^t ds \left\{ \exp -(t-s) \left[2\lambda + \frac{\partial}{\partial x} A(x) \right] \right\} \frac{\partial}{\partial x} g(x)p_s(x) \quad (69)$$

which has been the starting point of many recent model studies. 17-20) The stationary probability $\bar{p}(x)$ is obtained by integrating (69) from $s=0$ to $s=\infty$ and setting the probability current equal to zero. This yields

$$A(x) \bar{p}(x) = a_0^2 g(x) \left\{ \frac{1}{2\lambda + \frac{d}{dx} A(x)} \right\} \frac{d}{dx} (g(x)\bar{p}(x)), \quad (70)$$

which constitutes an implicit first order differential equation for $\bar{p}(x)$. Its solution reads

$$\bar{p}(x) = N^{-1} \frac{|g(x)|}{(a_0^2 g^2(x) - A^2(x))} \exp \left\{ 2\lambda \int^x dy \frac{A(y)}{(a_0^2 g^2(y) - A^2(y))} \right\}, \quad (71)$$

and is being defined in regions of x , where the denominator of the first term takes on positive values.

We conclude this article by pointing out that there exist of course alternative procedures for studying random dynamical systems which do not introduce the method of functional derivatives explicitly, but equivalent formal expressions instead. 21-24)

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