Correlation Functions and Masterequations of Generalized (Non-Markovian) Langevin Equations*

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For the statistical behavior of macrovariables described in terms of Langevin equations with a in general colored random force we deduce useful formulas which simplify the calculation of correlation functions. Utilizing these results and the stochastic properties of the random force we derive an exact time-convolutionless masterequation for the probability hereby showing the mathematical equivalence of the formally different approaches of a Langevin description and a masterequation description. We study in detail the class of time-instantaneous Langevin equations and the important class of retarded (Mori-type) Langevin equations with both, Gaussian and general colored random forces. Using the generalization of the nonlinear Langevin equation for continuous Markov processes with white Gaussian noise and white generalized Poisson noise we show that the resulting masterequation can be recast in the Kramers-Moyal form. Interpreting this Langevin equation in the Stratonovitch sense we deduce the fluctuation induced drift (spurious drift) which can be divided up into two parts, the well known part induced by white Gaussian noise and the one induced by white generalized Poisson noise.

1. Introduction

In the last years an ever increasing interest is paid to the modelling of statistical problems in equilibrium and nonequilibrium mechanics in terms of stochastic differential equations for the macrovariables (generalized Langevin equations). In principle all properties of the fluctuations are implied by the microscopic equations for all degrees of freedom. Using the powerful projection operator technique Mori [1] developed a formalism which leads to an exact stochastic differential equation, but with a random force whose properties are known only in the vicinity of the thermal equilibrum state. An attempt to states far from equilibrum has been put forward by various people [2-4]. In particular, Grabert [4] developed an exact equation for the fluctuations around the timedependent mean values. In all of these exact equations the non-Markovian character shows up clearly by the occurence of so called memory terms and

random forces with a colored correlation. In practice however, these exact Langevin equations involve many technical difficulties connected with the evaluation of the various transport quantities in such equations. An approach on an intermediate level, more detailed than the deterministic picture but less detailed than the microscopic one appears to be most fruitful. The way of computing fluctuations on such a "mesoscopic" level consists in approximations for the quantities in the exact equations but retaining the correct structure.

A well known approximation is the description of macrovariables in terms of continuous Markov processes modelled by Langevin equations with Gaussian white random forces [5, 6]. The equivalence of such a description and the corresponding masterequation, the Fokker-Planck equation is well known and represents a widely used concept [5, 6]. However, the physical justification for such an approximation is often dubious and not well understood. For example, even a modelling of physical system with a Langevin

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equation which is mathematically equivalent to a masterequation of a Markov process $\mathbf{x}(t)$ in the form of an infinite order differential operator (Kramers-Moyal expansion [7]) has not been considered in detail so far. Because of the large variety of factors responsible for the fluctuations, more satisfactory is that approach implying for the description of the system continuous or discontinuous sample paths generated from colored Markovian or non-Markovian driving forces.

In order not to complicate the main ideas we restrict in the following the discussion to statistical systems described in terms of a single collective variable z(t)driven by one stochastic (in general non-Markovian) random force. For the stochastic differential equation we have in general a structure of the form

$$\dot{z}(t) = \alpha(t) \, z(t) + \beta(z(t), t) \int_{0}^{t} z(s) \, d\Gamma(t, s) + f(t),$$

$$t \ge 0.$$
(1.1)

Here the random force f(t) may depend in general on the macrovariable z(t) itself. For example the fluctuating force in the Mori-theory [1–2] for the thermal equilibrium is orthogonal only to the first power of the macrovariable and thus includes terms nonlinear in the collective variable. Note that with the choice $\Gamma(t,s) = \Theta(t-s^+)$ we obtain a time-instantaneous stochastic differential equation with the structure

$$\dot{z}(t) = a(z,t) + f(t).$$
 (1.2)

Setting $d\Gamma(t, s)$ equal to $\gamma(t-s)ds$ and $\beta(z, t)$ equal to 1 we obtain from (1.1) the linear non-Markovian generalized Langevin equation of the Mori-type. A third class of dynamical systems modelled by (1.1) is obtained setting $\Gamma(t, s) = \Theta(s - (t - T))$ with T a fixed time-lag. This class of systems plays an important role in biophysical problems [8], e.g. for the behavior of the dynamics of antigen-antibody reactions [8,9]. Our concern in this paper will be to investigate the calculation of correlation functions of the process z(t)described by a stochastic differential equation of the form in (1.1) and to derive an exact masterequation describing the rate of change of the macroprobability function p(z, t).

The paper is organized as follows. Noting that the solutions of (1.1) are functionals of the random force f(t) we deduce simple formulas for the calculation of a correlation function

$$\langle z(r) g(\{z(s), 0 \le s \le t\}) \rangle. \tag{1.3}$$

Such correlation functions play a major role in the calculation of various transport coefficients. Mo-

reover, the study of the correlation functions in (1.3) specify to a certain degree the nature of the stochastic process under consideration. Section 3 contains the main results of this paper. Given the knowledge of the initial probability p_0 and the stochastic properties (cumulants) of the random force f(t) we derive an exact time-convolutionless equation for the rate of change of the probability p(z, t) having the form of a masterequation with a in general p_0 -dependent generator $\Gamma(t)$

$$\dot{p}(t) = \Gamma(t) p(t). \tag{1.4}$$

In particular, we study in detail the stochastic operator $\Gamma(t)$ for generalized Langevin equations of the form in (1.2) and for linear generalized non-Markovian Langevin equations of the Mori-type. Under special assumptions stated in Section 3, the generator becomes even a linear operator (i.e. p_0 -independent). But this does not mean that the process z(t) is now a Markov process [10]. The limiting case of a nonlinear generalized Langevin equation of the form in (1.2) with in each point independent continuous and discontinuous increments is shown to be equivalent to the master-equation of a Markov process z(t) in the form of the Kramers-Moyal expansion [7]. Using the Stratonovitch interpretation for this generalized Langevin equation we derive the fluctuation induced drift terms (spurious drift) of both, the well known part induced by the continuous increments and the part induced by the *discontinuous* increments.

2. Characteristic Functionals and Correlation Functions

Let us first expand the concept of usual probability theory a little bit further. We permit to ask the following question: What is the probability of obtaining the particular time history of a physical phenomenon described by an equation like (1.1). Thus we are led to consider the probability of functions in a certain class (the probability of a single realization has a vanishing measure). Hence, we write for the probability of finding the function in a specified class A of functions with help of a probability functional p(z(t))

$$\int_{A} p(z(t)) \mathcal{D} z(t). \tag{2.1}$$

In an analogous fashion to usual probability techniques the mean value of a functional Q(z(t)) is written as

$$\langle Q(z) \rangle = \int Q(z(t)) p(z(t)) \mathcal{D} z(t) / \int p(z(t)) \mathcal{D} z(t).$$
 (2.2)

A very useful mean value of a functional is the moment generating functional, the characteristic functional $\Phi[v]$ [11] defined by

$$\Phi[v] = \langle \exp i \int ds \, v(s) \, z(s) \rangle, \quad \Phi[v=0] = 1.$$
(2.3)

The expansion of $\Phi[v]$ in a functional Taylor series determines the *n*-(time) point moments

$$\Phi[v] = \sum_{n=0}^{\infty} \frac{(i)^n}{n!} \int d\mathbf{t} \, m_n(t_1, \dots t_n) \, v(t_1) \dots \, v(t_n), \qquad (2.4)$$

$$m_{n} \equiv m_{n}(t_{1}, \dots, t_{n}) = \langle z(t_{1}) \dots z(t_{n}) \rangle$$

= $(i)^{-n} \frac{\delta^{n}}{\delta_{v}(t_{1}) \dots \delta v(t_{n})} \Phi[v]|_{v=0}.$ (2.5)

The notation $\int dt$ in (2.4) denotes the multidimensional integral $\int \dots \int dt_1 \dots dt_n$. We remark that the moment m_n is a symmetric function with respect to its time-arguments. It is often convenient to work with the cumulant generating functional $\Psi[v]$

$$\Psi[v] = \ln \Phi[v]. \tag{2.6}$$

An expansion in a functional Taylor series defines the n-point cumulants K_n

$$\Psi[v] = \sum_{n=1}^{\infty} \frac{(i)^n}{n!} \int d\mathbf{t} \, K_n(t_1, \dots, t_n) \, v(t_1) \dots \, v(t_n), \qquad (2.7)$$

with

$$K_n = K_n(t_1, \dots, t_n) = (i)^{-n} \cdot \frac{\partial^n}{\delta v(t_1) \dots \delta v(t_n)} \Psi[v]|_{v=0}.$$
(2.8)

The main purpose in this section is to derive some *practical* formulas for the calculation of a general correlation function of the form

$$\langle z(t) g(\{z(\tau), 0 \le \tau \le t_f\}) \rangle,$$
 (2.9)

where g(z) is some functional of the stochastic process z(t). For the evaluation of (2.9) we make use of the well known trick of the introduction of a auxiliary functional $g(z+\eta)$ with η a determined arbitrary function which is set equal to zero in the final formulas. Expanding $g(z+\eta)$ in a functional Taylor series in z we obtain for the correlation in (2.9)

$$\langle z(t) g(z+\eta) \rangle$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \int d\mathbf{t} \frac{\delta^n g(\eta)}{\delta \eta(t_1) \dots \delta \eta(t_n)} \langle z(t_1) \dots z(t_n) z(t) \rangle$$
(2.10)
$$= \sum_{n=0}^{\infty} \frac{1}{(i)^{n+1} n!} \int d\mathbf{t} \frac{\delta^n g(\eta)}{\delta \eta(t_1) \dots \delta \eta(t_n)}$$

$$\cdot \frac{\delta^n}{\delta v(t_1) \dots \delta v(t_n)} \frac{\delta \Psi}{\delta v(t)} \Phi|_{v=0}$$
(2.11)
$$= \sum_{n=0}^{\infty} \sum_{j=0}^{n} \frac{1}{j! (n-j)!} \int d\mathbf{t} \frac{\delta^n g(\eta)}{\delta \eta(t_1) \dots \delta \eta(t_n)}$$

$$\cdot K_{j+1}(t, t_1 \dots t_j) m_{n-j}(t_{j+1}, \dots t_n).$$
 (2.12)

In (2.12) we made use of the Leibnitz rule for the (functional) product differentiation $\left[\Phi\left(\frac{\delta\Psi}{\delta v}\right)\right]^{(n)}$. If we change the order of summation in (2.12) and observe the expression for the Taylor expansion of $g(z+\eta)$ in z we find by setting $\eta=0$ the useful expression

$$\langle z(t) g(z) \rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int d\mathbf{t} K_{n+1}(t, t_1 \dots t_n) \cdot \left\langle \frac{\delta^n g(z)}{\delta z(t_1) \dots \delta z(t_n)} \right\rangle.$$
(2.13)

This result can be rewritten in compact form by use of the auxiliary functional $\Omega_t[v]$

$$\Omega_{t}[v] = \frac{\delta \Psi}{i \, \delta v(t)}$$

$$= \sum_{n=1}^{\infty} \frac{(i)^{n-1}}{(n-1)!} \int d\mathbf{t} \, K_{n}(t, t_{1}, \dots, t_{n-1}) \, v(t_{1}) \dots \, v(t_{n-1})$$

$$= \sum_{m=0}^{\infty} \frac{i^{m}}{m!} \int d\mathbf{t} \, K_{m+1}(t, t_{1}, \dots, t_{m}) \, v(t_{1}) \dots \, v(t_{m}) \qquad (2.14)$$

yielding*

$$\langle z(t) g(z) \rangle = \left\langle \Omega_t \left[\frac{\delta}{i \, \delta z} \right] g(z) \right\rangle.$$
 (2.15)

As a byresult of (2.15) we obtain for the functional $g(z) = z(t_1) \dots z(t_{n-1})$ a recursive relationship between the *n*-point correlation $m_n(t_1, \dots, t_{n-1}, t)$ and the cumulants of z(t)

$$\langle z(t_1) \dots z(t_{n-1}) z(t) \rangle - \langle z(t) \rangle \langle z(t_1) \dots z(t_{n-1}) \rangle$$

= $\sum_{i=1}^{n-1} \frac{1}{i!} \int d\mathbf{s} \, K_{i+1}(t, s_1, \dots s_i) \left\langle \frac{\delta^i z(t_1) \dots z(t_{n-1})}{\delta z(s_1) \dots \delta z(s_i)} \right\rangle.$ (2.16)

Note that from a physical point of view the history of the sample functions generated by the stochastic differential equation is known only in the interval [0, t]! For the description of the statistical process z(s), $0 \le s \le t$ it is therefore oppertune to introduce for the following the "trimed" characteristic functional $\Phi_t[v]$

$$\Phi_t[v] = \left\langle \exp i \int_0^t ds \, v(s) \, z(s) \right\rangle, \quad \Phi_t[v=0] = 1, \quad (2.17)$$

and correspondingly

$$\Psi_t[v] = \ln \Phi_t[v]. \tag{2.18}$$

* In case that z(t)=z is a random variable the result in (2.15) yields many practical formulas, e.g. for

$$\langle z g(z) \rangle = \sum_{n=0}^{\infty} \frac{1}{n!} K_{n+1} \left\langle \frac{d^n g(z)}{dz^n} \right\rangle$$

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These functionals are obtained from the old ones by the substitution $v(s) \rightarrow \Theta(s) \Theta(t-s) v(s)$. $\Theta(s)$ denotes the usual unit step function.

For all correlations $\langle z(t')g(z)\rangle$ in which $0 \leq t' < t$ the above results remain true, i.e. for t' < t and z(s), $0 \leq s \leq t$ we can write for (2.13)

$$\langle z(t') g(z) \rangle$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \int_{0}^{t} d\mathbf{t} K_{n+1}(t', t_{1}, \dots, t_{n}) \left\langle \frac{\delta^{n} g(z)}{\delta z(t_{1}) \dots \delta z(t_{n})} \right\rangle$$
(2.19)
$$= \left\langle \Omega_{t,t'} \left[\frac{\delta}{i \, \delta z} \right] g(z) \right\rangle.$$

$$(2.20)$$

But now the case where t' = t needs in general (e.g. δ correlated processes) a special investigation. Expanding again $g(z+\eta)$ in a functional Taylor series in z we obtain with (2.17)

$$\langle z(t) g(z+\eta) \rangle$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \langle i \rangle^{-n} \int_{0}^{t} dt \frac{\delta^{n} g(\eta)}{\delta \eta(t_{1}) \dots \delta \eta(t_{n})}$$

$$\cdot \frac{\delta^{n}}{\delta v(t_{1}) \dots \delta v(t_{n})} \left\{ \frac{1}{i v(t)} \left[\frac{\partial}{\partial t} \ln \Phi_{t} [v] \right] \Phi_{t} [v] \right\} \Big|_{v=0}.$$
(2.21)

By virtue of the auxiliary functional $\Sigma_t[v]$

$$\Sigma_{t}[v] = \frac{1}{i v(t)} \frac{\partial}{\partial t} \ln \Phi_{t}[v]$$

$$\equiv \sum_{n=0}^{\infty} \frac{(i)^{n}}{n!} \int_{0}^{t} dt C_{n}(t, t_{1} \dots t_{n}) v(t_{1}) \dots v(t_{n}) \qquad (2.22)$$

(2.21) becomes

 $\langle z(t) g(z+\eta) \rangle$

$$= \sum_{n=0}^{\infty} \sum_{k=0}^{\infty} \frac{\int d\mathbf{t}}{k!(n-k)!} \int_{0}^{\infty} d\mathbf{t} \frac{\delta(n)}{\delta \eta(t_1) \dots \delta \eta(t_n)}$$

$$\cdot C_k(t, t_1, \dots t_k) m_{n-k}(t_{k+1}, \dots t_n)$$
(2.23 a)

 $\delta^n g(\eta)$

$$=\sum_{k=0}^{\infty} \frac{1}{k!} \int_{0}^{t} d\mathbf{t} C_{k}(t,t_{1},\ldots,t_{k}) \frac{\delta^{k}}{\delta\eta(t_{1})\ldots\delta\eta(t_{k})}$$
$$\cdot \sum_{n=0}^{\infty} \frac{1}{n!} \int_{0}^{t} d\mathbf{s} \frac{\delta^{n} g(\eta)}{\delta\eta(s_{1})\ldots\delta\eta(s_{n})} m_{n}(s_{1},\ldots,s_{n})$$
(2.23b)

$$=\sum_{k=0}^{\infty} \frac{1}{k!} \int_{0}^{t} dt_{1} \dots \int_{0}^{t} dt_{k} C_{k}(t, t_{1}, \dots, t_{k})$$
$$\cdot \left\langle \frac{\delta^{k} g(z+\eta)}{\delta \eta(t_{1}) \dots \delta \eta(t_{k})} \right\rangle.$$
(2.23c)

Whence by setting $\eta = 0$ we have for t' = t the final result

$$\langle z(t) g(z) = \left\langle \Sigma_t \left[\frac{\delta}{i \, \delta z} \right] g(z) \right\rangle.$$
 (2.24)

The deduced formulas in (2.19), (2.20) and (2.24)simplify considerably the calculation of correlation functions of the process z(s) with a functional g(z). As we shall see, they play an important role for the derivation of masterequations of stochastic processes described by generalized Langevin equations. Applications of the derived formulas for a general Gaussian process, for the generalized Poisson process and for white Gaussian and white generalized Poisson processes are given in the Appendix. The latter class of white processes plays an important role for the description of Markov processes in terms of Langevin equations.

3. Masterequations for Generalized Langevin Equations

The single-event masterequation for the process z(t) provides a powerful tool for the calculation of a general relaxation function $\langle F(z(t)) \rangle$. Moreover, the concept of the masterequation elucidates the problem of the equivalence of a statistical description either in terms of a masterequation or a generalized Langevin equation. To start with, suppose we deal with the general stochastic differential equation for z(t) in equation (1.1) with the random force in the form $f(t) \rightarrow b(z, t) f(t)$

$$\dot{z}(t) = \alpha(t) z(t) + \beta(z(t), t)$$

$$\cdot \int_{0}^{t} \gamma(t, s) z(s) ds + b(z(t), t) f(t), \quad t > 0$$

$$z(0) = z_{0}. \quad (3.1)$$

The probability density p(z, t) can be written in terms of the expectation

$$p(z,t) = \langle \delta(z(t) - z) \rangle. \tag{3.2}$$

Note that the average in (3.2) is over all the realizations of the stochastic driving force f(t) and over the initial probability $p_0(z)$ of the distributed starting value z_0 . By differentiation of the equal time correlation (3.2) with respect to the parameter t we obtain

$$\dot{p}(z,t) = -\alpha(t) \frac{\partial}{\partial z} z \, p(z,t) - \frac{\partial}{\partial z} \beta(z,t) \left\langle \int_{0}^{t} ds \, \gamma(t,s) \, z(s) \, \delta(z(t)-z) \right\rangle - \frac{\partial}{\partial z} b(z,t) \left\langle \Sigma_{t} \left[\frac{\delta}{i \, \delta f} \right] \delta(z(t)-z) \right\rangle.$$
(3.3)

Because the process z(t) is a functional of the random force f(s) we could use the result in (2.24) for the correlation $\langle f(t)b(z(t),t)\delta(z(t)-z)\rangle$ that occurs in the last term of (3.3). Equation (3.3) is an exact kinetic equation for the probability p(z, t) of the non-Markov process z(t). Let us comment some more about the structure of (3.3): It is not a closed expression for the probability due to the memory expressions in the last two terms. The equation is also nonlinear in the sense that the average in the second and third term may be explicitly dependent on the chosen initial probability p_0 . Even the random force f(t) may in general have different stochastic properties for different chosen preparation procedures for the physical system [12]and choice of the initial probability $p_0(z)$. For example, if $\langle f(t) \rangle$ is zero for one choice of p_0 it is not, in general, for a different choice \bar{p}_0 . Henceforth, the functional Σ_t represents in general a process-dependent operator. Note also, provided (3.1) is supplemented by a deterministic part

$$\dot{\mathbf{y}}(t) = \mathbf{c}(\mathbf{x}, t), \tag{3.4}$$

where x denotes the vectorial process $\mathbf{x}(t) = (\mathbf{y}(t), z(t))$ the masterequation for the process $\mathbf{x}(t)$ has the structure of (3.3) augmented simply by the term

$$-\nabla \mathbf{c}(\mathbf{x},t) \, p(\mathbf{x},t). \tag{3.5}$$

In order to discuss the kinetic equation for p(z, t) in more detail we consider the following classes of generalized Langevin equations.

3.1. Time-Instantaneous Generalized Langevin Equations

In case that $\gamma(t, s)$ in (3.1) is of the form

$$\gamma(t,s) = \gamma(t)\,\delta(t-s^+) \tag{3.6}$$

we obtain the time-instantaneous generalized Langevin equation in (1.2)

$$\dot{z}(t) = a(z,t) + b(z,t)f(t).$$
 (3.7)

It is worth emphasizing at this stage the following: As long as the stochastic force in (3.7) is not specified further the memory-less (often called "markovian") form of (3.7) does of course not imply that we deal with a Markovian process z(t)! For the masterequation of the processes described by (3.7) we obtain from (3.3)

$$\dot{p}(z,t) = -\frac{\partial}{\partial z} a(z,t) p(z,t) -\frac{\partial}{\partial z} b(z,t) \left\langle \Sigma_t \left[\frac{\delta}{i \, \delta f} \right] \delta(z(t) - z) \right\rangle.$$
(3.8)

$$\dot{z}(t) = \alpha(t) z(t) + v(t),$$
 (3.9)

with the redefined random force

$$v(t) = a(z, t) - \alpha(t) z(t) + b(z, t) f(t).$$
(3.10)

As a consequence, this random force v(t) contains macroscopic processes through the nonlinear terms. Thus, the correlation $\langle v(t) v(s) \rangle$ has in general a macroscopic longlived time-scale. For linear systems this random force may often be well approximated by a δ -correlated random force v(t). By use of the in general process dependent auxiliary functional $\Sigma_t^{(v)}$ formed with the cumulants of v(t) (3.8) becomes

$$\dot{p}(z,t) = -\alpha(t) \frac{\partial}{\partial z} z \, p(z,t) - \frac{\partial}{\partial z} \left\langle \Sigma_t^{(v)} \left[\frac{\delta}{i \, \delta v} \right] \delta(z(t) - z) \right\rangle.$$
(3.11)

Observing the dynamical nature of z(t) in (3.9) we obtain for the functional derivative

$$\frac{\delta}{\delta v(s)} \delta(z(t) - z) = -\left(\frac{\delta z(t)}{\delta v(s)}\right) \frac{\partial}{\partial z} \delta(z(t) - z).$$
$$= \exp \int_{-\infty}^{t} \alpha(r) dr \frac{-\partial}{\partial z} \delta(z(t) - z), \qquad (3.12)$$

which combines with (3.11) to an exact time-convolutionless closed masterequation

$$\dot{p}(z,t) = -\alpha(t)\frac{\partial}{\partial z}z \,p(z,t) -\frac{\partial}{\partial z}\Sigma_t^{(\nu)} \left[i\exp\int_{s}^{t}\alpha(r)\,dr\frac{\partial}{\partial z}\right]p(z,t).$$
(3.13)

This closed masterequation is a first central result of this work. The fact that the operator $\Sigma_t^{(v)}$ is generally process dependent (i.e. depends via the cumulants of v(t) on the chosen initial probability p_0) clearly reflects the non-Markovian character of the process z(t). Further, assuming that the random force v(t) has statistical properties which do not depend on p_0 (e.g. if v(t) is a z-independent colored Gaussian process) the masterequation in (3.13) becomes a *linear* closed operator equation for p(z, t)

$$\dot{p}(t) = \Gamma(t) p(t), \qquad (3.14)$$

with

$$\Gamma(t) = -\alpha(t)\frac{\partial}{\partial z}z - \frac{\partial}{\partial z}\Sigma_t^{(\nu)}\left[i\exp\int_s^t \alpha(r)\,dr\,\frac{\partial}{\partial z}\right].\tag{3.15}$$

Thus, the solution of (3.14) can be written in terms of a linear propagator set $\{G(t|s), t > s\}$.

$$p(t) = G(t|s) p(s), \quad t > s,$$
 (3.16)

with

$$G(t|s) = \mathscr{T} \exp \int_{s} \Gamma(r) dr.$$
(3.17)

 \mathcal{T} means the usual time-ordering operator. The kernels of these propagators satisfy a (pseudo-) Kolmogororov equation

$$G(t|t_1) = G(t|s) G(s|t_1), \quad t \ge s \ge t_1.$$
(3.18)

Note that for the special time set [0, t] the kernel of the propagator G(t|0) coincides in this case with the initial conditional probability R(t|0) of the process z(t) (for details of this conclusion see Ref. [10]):

$$G(z t | z_0 0) = R(z t | z_0 0).$$
(3.19)

As a consequence, the linear closed masterequation (3.16) determines over R(t|0) the dynamics of initial correlation functions C(t, 0)

$$C(t, 0) = \langle F(z(t)) H(z(0)) \rangle, \quad t > 0.$$
 (3.20)

In contrast to the Markov case, this does not hold for aged correlation functions C(t, s), s > 0 [10, 12].

As one example for (3.15) we consider the stochastic differential equation in (3.9) with a colored z-independent Gaussian random force defined by

$$\langle v(t) \rangle = m(t),$$
 (3.21)

and

$$\langle v(t)v(s)\rangle = \sigma(t,s) + m(t)m(s).$$
 (3.22)

Using the result in (A.3) for Σ_t we obtain immediately for the masterequation the "Fokker-Planck type" equation

$$\dot{p}(z,t) = -\alpha(t)\frac{\partial}{\partial z}z\,p(z,t) - m(t)\frac{\partial}{\partial z}p(z,t) + \left\{\int_{0}^{t} ds\,\sigma(t,s)\exp\int_{s}^{t}\alpha(r)\,dr\right\}\frac{\partial^{2}}{\partial z^{2}}p(z,t).$$
(3.23)

Another class of processes yielding always a closed operator expression for the rate of change of p(z, t) without utilizing the concept in (3.9) is obtained if f(t) in (3.1) is for all cumulants K_n , n > 1 (K_n may be still p_0 -dependent) a δ -correlated random process. Then we have in a handy-dandy notation

$$\Sigma_t \left[\frac{\delta}{i \, \delta f(s)} \right] = \Sigma_t \left[\frac{\delta}{i \, \delta f(t)} \right]. \tag{3.24}$$

and

$$b(z,t)\frac{\delta}{\delta f(t)}\delta(z(t)-z) = -b(z,t)\frac{\partial}{\partial z}b(z,t)\,\delta(z(t)-z).$$
(3.25)

Here we made use of the exact relation

$$\frac{\delta z(t)}{\delta f(s)} = b(z(s), s) + \int_{s}^{t} d\tau \left\{ \frac{\partial}{\partial z} a(z, \tau) + \frac{\partial}{\partial z} b(z, \tau) f(\tau) \right\} \frac{\delta z(\tau)}{\delta f(s)}$$
(3.26)

for the parameter choice s = t.

Observing (3.25) the master equation in (3.8) can be rewritten in a closed form

$$\dot{p}(z,t) = -\frac{\partial}{\partial z}a(z,t) p(z,t)$$

$$-\frac{\partial}{\partial z}\Sigma_t \left[i b(z,t)\frac{\partial}{\partial z}\right]b(z,t) p(z,t). \qquad (3.27)$$

This equation represents a second main result. The assumption of δ -correlated noise in nonlinear statistical problems can be justified in many cases after a partial coarse graining in space and time has been performed $\lceil 1-2 \rceil$.*

As a special application we consider those processes for which z(t) is composed of in each time-point independent increments. Only in this case it is guaranteed that z(t) is a Markov process [16]! This point has not been paid attention in a recent paper [13] showing a possible equivalence between a generalized Langevin equation and the masterequation for Markov processes z(t). Decomposing the random force in (3.1) into the two terms

$$b(z,t)f(t) = \gamma_{G}(z,t)\,\zeta_{G}(t) + \gamma_{P}(z,t)\,\zeta_{P}(t), \qquad (3.28)$$

where $\xi_G(t)$ denotes a normalized white Gaussian process, (A.6), and $\xi_P(t)$ a white generalized Poisson process, (A.16), the solution of (3.7) describes a *Markov process* z(t). For the masterequation we obtain by use of the expressions in (A.8) and (A.18) the general Kolmogorov-Feller equation

$$\dot{p}(z,t) = -\frac{\partial}{\partial z} a(z,t) p(z,t)$$

$$+ 1/2 \frac{\partial}{\partial z} \gamma_G(z,t) \frac{\partial}{\partial z} \gamma_G(z,t) p(z,t)$$

$$- \frac{\partial}{\partial z} \left\{ \lambda \int_{-\infty}^{+\infty} dx \, q(x) \int_{0}^{x} du \exp\left[-u \gamma_P(z,t) \frac{\partial}{\partial z}\right] \right\}$$

$$\cdot \gamma_P(z,t) \, p(z,t), \qquad (3.29 a)$$

$$= -\frac{\partial}{\partial z} a(z,t) \, p(z,t) + 1/2 \left(\frac{\partial}{\partial z} \gamma_G(z,t)\right)^2 p(z,t)$$

$$+ \lambda \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} \langle x^n \rangle \left(\frac{\partial}{\partial z} \gamma_P(z,t)\right)^n p(z,t), \quad \langle x \rangle = 0.$$

$$(3.29 b)$$

^{*} Though the stochastic properties for the higher cumulants are set up beyond all physical intuition they are often a consequence of the nature of approximation used for the lower cumulants

Here q(x) denotes the probability of the statistically independent jump random variables in the generalized Poisson process and λ is the parameter in the Poisson counting process. This masterequation can be recast in the Kramers-Moyal form [7]

$$= -\frac{\partial}{\partial z} \left[a(z,t) + 1/2 \gamma_G(z,t) \frac{\partial \gamma_G(z,t)}{\partial z} \right] p(z,t) + 1/2 \frac{\partial^2}{\partial z^2} \gamma_G^2(z,t) p(z,t) + \lambda \sum_{k=1}^{\infty} (-1)^k \left(\frac{\partial}{\partial z} \right)^k \cdot \left(\sum_{n=\max(k,2)}^{\infty} 1/n ! \langle x^n \rangle \gamma_P(z,t) D^{n-k} [\gamma_P^{n-1}(z,t)] \right) p(z,t)$$
(3.30a)

$$=\sum_{n=1}^{\infty} (-1)^n / n! \left(\frac{\partial}{\partial z}\right)^n [c_n(z,t) p(z,t)], \qquad (3.30b)$$

where the moments are given by

$$c_{1} = a(z, t) + 1/2 \gamma_{G} \frac{\partial \gamma_{G}}{\partial z} + \lambda \sum_{n=2}^{\infty} 1/n! \langle x^{n} \rangle \gamma_{P} D^{n-1} [\gamma_{P}^{n-1}], \qquad (3.31)$$

$$c_{2} = \gamma_{G}^{2} + 2\lambda \sum_{n=2}^{\infty} 1/n! \gamma_{P} D^{n-2} [\gamma_{P}^{n-1}], \qquad (3.32)$$

$$c_{n} = n ! \lambda \sum_{m=n}^{\infty} 1/m ! \langle x^{m} \rangle \gamma_{P} D^{m-n} [\gamma_{P}^{m-1}],$$

$$n > 2.$$
(3.33)

Hereby we made use of the functional D^{j} introduced by Bedeaux [13]

$$D^{J}[\gamma_{P}^{n}(z,t)] = \sum_{i_{1},\ldots,i_{j+1}}^{n} \left[\gamma_{P}^{i_{1}} \frac{\partial}{\partial z} \gamma_{P}^{i_{2}} \frac{\partial}{\partial z} \ldots \gamma_{P}^{i_{j+1}} \right].$$

$$i_{1} + \cdots + i_{j+1} = n, \quad 0 \leq i_{k} \leq n$$
(3.34)

Note that this functional acts only upon the functions between the square brackets yielding as result a function. Hence, we have shown that a generalized Langevin equation of the form in (3.7) with the random force in (3.28) is mathematically equivalent to a masterequation in (3.29) or (3.30) for the Markov process z(t). Furthermore, the kernel of the propagator for (3.30), G(xt|ys), t > s coincides with the conditional probability R(x t | y s), t > s for arbitrary aged times t, s so that the full dynamics of the Markovprocess is contained in (3.30) with knowledge of the initial probability p_0 . The first two terms in (3.30) just make up the well known Fokker-Planck equation for continuous Markov processes z(t) if we interpret the generalized Langevin equation, [(3.7) with (3.28)], in the Stratonovitch sense. This is in agreement with the theorem of Clark [14] and Wong and Zakai [15, 16] to white noise in the Langevin equation leads to the Stratonovitch definition. Equation (3.31) includes the fluctuation induced (Stratonovitch-) drift (or spurious drift) divided up into two parts, the well known part induced by white Gaussian noise and the one induced by white generalized Poisson noise. They naturally vanish if γ_G and γ_P are chosen z-independent.

3.2. Linear Non-Markovian Generalized Langevin Equations

An important role in the theory of statistical mechanics play the linear non-Markovian Langevin equations of the Mori form [1-4]:

$$\dot{z}(t) = -\int_{0}^{t} \gamma(t-s) \, z(s) \, ds + f(t) \tag{3.35}$$

where the memorykernel $\gamma(t-s)$ may contain in general an instantaneous contribution

$$a\,\delta(t-s^+).\tag{3.36}$$

Though it is in practice no easy matter to obtain the statistical properties of the random force f(t) form first principles they are assumed to be known (at least formally) for the following. By use of the function $\chi(t)$ obeying

$$\dot{\chi}(t) = -\int_{0}^{t} \gamma(t-s) \,\chi(s) \, ds, \qquad \chi(0) = 1, \tag{3.37}$$

we obtain for the solution of (3.35) with the initial probability $p_0(z) = \delta(z - z_0)$

$$z(t) = \chi(t) z_0 + \int_0^t \chi(t-s) f(s) \, ds.$$
(3.38)

We remark that only under the additional assumption

$$\langle f(t) z_0 \rangle = 0, \tag{3.39}$$

the function $\chi(t)$ coincides with the *initial* correlation function

$$\chi(t) = \langle z(t) \, z(0) \rangle / \langle z^2(0) \rangle. \tag{3.40}$$

By virtue of the equations (3.3), (3.20), (3.38) and the relation

$$\frac{\delta}{\delta f(u)}\delta(z(t)-z) = -\chi(t-u)\frac{\partial}{\partial z}\delta(z(t)-z)$$
(3.41)

we obtain for the masterequation of z(t) under the initial condition $p_0(z) = \delta(z - z_0)$ the closed equation

$$\dot{p}(z,t) = z_0 \int_0^t \gamma(t-s) \chi(s) \, ds \, \frac{\partial}{\partial z} p(z,t) + \int_0^t ds \, \gamma(t-s) \int_0^s dr \, \chi(s-r) \, \frac{\partial}{\partial z} \Omega_{t,r} \left[i \, \overline{\chi} \, \frac{\partial}{\partial z} \right] p(z,t) - \frac{\partial}{\partial z} \Sigma_t \left[i \, \overline{\chi} \, \frac{\partial}{\partial z} \right] p(z,t),$$
where $\overline{\chi}(u) = \chi(t-u).$ (3.42)

This is an exact closed time-convolutionless masterequation for Mori-type Langevin equations which depends through the initial probability $p_0(z) = \delta(z - z_0)$ explicitly on z_0 . The remaining terms may also depend on p_0 via the cumulants of f(t) in the operator functionals $\Omega_{t,r}$ and Σ_t (c.f. (2.19) and the Appendix). For the following we assume that in the exact Langevin equation (3.35) a partial coarse graining in time has been performed such that the "correlation" $\chi(t)$ takes on only positive values for finite times t. Expressing z_0 with help of (3.38), the generalized Langevin equation (3.35) can then be transformed into an exact time-convolutionless form

$$\dot{z}(t) = (\dot{\chi}(t)/\chi(t)) z(t) - (\dot{\chi}(t)/\chi(t)) \int_{0}^{t} \chi(t-s) f(s) ds$$

+ $\int_{0}^{t} \dot{\chi}(t-s) f(s) ds + f(t),$
= $\frac{d \ln \chi(t)}{dt} z(t) + \chi(t) \frac{d}{dt} \int_{0}^{t} \frac{\chi(t-s)}{\chi(t)} f(s) ds.$ (3.43)

Moreover, in presence of an external deterministic force F(t), coupled additively into (3.35), the perturbed total generalized Langevin equation reads

$$\dot{z}(t) = \frac{\dot{\chi}(t)}{\chi(t)} z(t) + \chi(t) \frac{d}{dt} \int_{0}^{t} \frac{\chi(t-s)}{\chi(t)} f(s) ds$$
$$+ \chi(t) \frac{d}{dt} \int_{0}^{t} \frac{\chi(t-s)}{\chi(t)} F(s) ds.$$
(3.44)

Thus, we have for the masterequation of the total perturbed system by use of (3.44) and the results in section 2 the closed equation

$$\dot{p}(z,t) = -(\dot{\chi}(t)/\chi(t))\frac{\partial}{\partial z}z \, p(z,t) + \frac{\dot{\chi}(t)}{\chi(t)} \int_{0}^{t} ds \, \chi(t-s)\frac{\partial}{\partial z} \Omega_{t,s} \left[i \bar{\chi} \frac{\partial}{\partial z} \right] p(z,t) - \int_{0}^{t} ds \, \dot{\chi}(t-s)\frac{\partial}{\partial z} \Omega_{t,s} \left[i \bar{\chi} \frac{\partial}{\partial z} \right] p(z,t) - \frac{\partial}{\partial z} \Sigma_{t} \left[i \bar{\chi} \frac{\partial}{\partial z} \right] p(z,t) - \chi(t) \left(\frac{d}{dt} \int_{0}^{t} \frac{\chi(t-s)}{\chi(t)} F(s) \, ds \right) \frac{\partial}{\partial z} p(z,t).$$
(3.45)

The rigorous result in (3.45) becomes a *linear* masterequation if the cumulants of the random force f(t) as well as $\chi(t)$ do not depend on the choice for the initial probability p_0 . In such a case it is also reasonable to require that the random force does not depend on the external force F(t). Then, the effect of the external perturbation is represented in (3.45) by the last term only in the form of a linear functional which involves, in contrast to the Markov case, $(\chi(t) = \exp - c t)$, the whole previous history of F(s) as well. The generator $\Gamma(t)$ defined by (3.45) represents in general a differential operator of infinite order. Only for the case that f(t) is a z-independent Gaussian process, e.g.

$$\langle f(t) \rangle = 0, \tag{3.46}$$

$$\langle f(t)f(s)\rangle = \sigma(t,s),$$
 (3.47)

the linear generator $\Gamma(t)$ reduces to a differential operator $\Gamma_G(t)$ of second order

$$\Gamma_{G}(t) = -\frac{\dot{\chi}(t)}{\chi(t)} \frac{\partial}{\partial z} z - \frac{\dot{\chi}(t)}{\chi(t)} \int_{0}^{t} ds \,\chi(t-s)$$

$$\cdot \int_{0}^{t} dr \,\chi(t-r) \,\sigma(s,r) \,\frac{\partial^{2}}{\partial z^{2}}$$

$$+ \int_{0}^{t} ds \,\dot{\chi}(t-s) \int_{0}^{t} dr \,\chi(t-r) \,\sigma(s,r) \frac{\partial^{2}}{\partial z^{2}}$$

$$+ \int_{0}^{t} dr \,\chi(t-r) \,\sigma(t,r) \frac{\partial^{2}}{\partial z^{2}}$$

$$- \chi(t) \,\left(\frac{d}{dt} \int_{0}^{t} ds \,\frac{\chi(t-s)}{\chi(t)} F(s)\right) \frac{\partial}{\partial z}. \qquad (3.48)$$

Here we made use of the explicit forms of $\Omega_{t,s}$ and Σ_t for Gaussian processes given in (A.2) and (A.3). The result in (3.48) can be simplified more if the random force in (3.46) and (3.47) is a stationary Gaussprocess which satisfies the 2-nd fluctuation-dissipation theorem introduced by Kubo [17]

$$\langle f(t)f(s)\rangle = \langle z^2 \rangle_{st} \gamma(|t-s|).$$
 (3.49)

Because of the independence of f(t) on $z(t), \chi(t)$ becomes

$$\chi(t) = \langle z(t) \, z(0) \rangle_{st} / \langle z^2 \rangle_{st}. \tag{3.50}$$

The index (s t) in (3.49) and (3.50) denotes the average over the unperturbed, (F(s)=0), stationary non-Markov Gaussprocess z(t) obtained from (3.43) when for the initial probability p_0 a Gaussian with vanishing mean is chosen. A somewhat laborous evaluation (double Laplace transform) of the terms in (3.48) yields with (3.49) the simple result [10]

$$\Gamma_{G}(t) = -\frac{\dot{\chi}(t)}{\chi(t)} \left[\frac{\partial}{\partial z} z + \langle z^{2} \rangle_{st} \frac{\partial^{2}}{\partial z^{2}} \right]
-\chi(t) \left(\frac{d}{dt} \int_{0}^{t} ds \frac{\chi(t-s)}{\chi(t)} F(s) \right) \frac{\partial}{\partial z}.$$
(3.51)

4. Conclusions

In this paper we have derived various formulas which simplify the calculation of stochastic quantities of non-Markov processes described in terms of a generalized Langevin equation. In particular, the results in section 2 elucidate how general correlation functions can be expressed via the cumulants of the process. The derivation of an exact time-convolutionless masterequation for different classes of generalized Langevin equations (e.g. for the Mori-type form) shows the mathematical equivalence of the two formally different approaches of a Langevin description and a masterequation description. The derivation of the masterequation mainly uses the stochastic properties of the random force f(t) via its cumulants. Note that two types of averaging are necessary in the final formulas. The first type is with respect to the stochastic random force whereas the second type of averaging is with respect to the distributed initial starting value z_0 of the collective variable. Whence, the resulting masterequation will depend in general on the explicitly chosen probability p_0 . The way how the higher cumulants of the random driving force enter in the operator expression for the masterequation is exhibited in transparent form via the functionals Σ_t and $\Omega_{t,s}$ defined in Section 2.

We stress that our method of derivation of the masterequation does not introduce formally questionable concepts like the inverse of operators which may not exist. Henceforth, our technique is substantially different from the method of Stratonovitch for non-Markov processes [18, 19], where one starts from the Taylor series expansion for the characteristic function in terms of all higher unknown moments of the macrovariable itself and derives by use of the inverse of a p_0 -dependent operator a time-convolutionless masterequation. But this "nonlinear" masterequation is not equivalent to ours in general also p_0 -dependent masterequation in (3.13); simply because there exist many process dependent time-convolutionless masterequations for the non-Markov process z(t) [20].

The generalization of the usual Langevin equation for continuous Markov processes to general Markov processes using white Gaussian noise and white generalized Poisson noise enables a treatment of the fluctuations which is mathematically equivalent to a masterequation description in the Kramers-Moyal form. For example, the results of Leibowitz [21] for *linear* stochastic systems with δ -correlated shot noise are contained in equation (3.30) as a special case. As a consequence, van Kampens objection against the treatment of fluctuations with the Langevin method [6] is not justified, unless one utilizes the erroneous procedure to describe a discontinuous Markov pro415

cess in terms of of a Langevin equation for a continuous Markov process.

Appendix

Applications of the results in section 2 to some important processes:

For a general Gaussprocess with mean $\langle z(t) \rangle = a(t)$ and second cumulant $\sigma(t, s)$ the characteristic functional $\Phi_t[v]$ reads [11]

$$\Phi_{t}[v] = \exp i \int_{0}^{t} v(s) a(s) ds$$

$$\exp - \frac{1}{2} \int_{0}^{t} \int_{0}^{t} v(s) v(r) \sigma(s, r) ds dr.$$
 (A.1)

Performing out the functional derivative $\delta \ln \Phi_t / i \, \delta v(s)$ we obtain for the auxiliary functional $\Omega_{t,s}[v]$

$$\Omega_{t,s}[v] = a(t) + i \int_{0}^{t} dr \,\sigma(s,r) \,v(r), \qquad (A.2)$$

and for $\Sigma_t[v] = 1/(iv(t)) \frac{\partial}{\partial t} \Psi_t[v]$ respectively

$$\Sigma_t[v] = \Omega_{t,s}[v]|_{s=t} = a(t) + i \int_0^t dr \,\sigma(t,r) \,v(r). \tag{A.3}$$

Whence, the correlation in (2.9) emerges as

$$\langle z(t') g(\{z(\tau), 0 \le \tau \le t\}) \rangle$$

$$= a(t') \langle g(\{z(\tau), 0 \le \tau \le t\}) \rangle$$

$$+ \int_{0}^{t} ds \, \sigma(t', s) \left\langle \frac{\delta g(z)}{\delta z(s)} \right\rangle.$$
(A.4)

Of interest in the theory of continuous Markov processes is the white Gaussian noise, i.e.

$$\langle z(t) \rangle = 0 \tag{A.5}$$

$$\langle z(t) z(s) \rangle = \sigma(t) \,\delta(t-s).$$
 (A.6)

From the above formulas (A.2) and (A.3) we obtain

$$\Omega_{s}[v] = i \sigma(s) v(s) \tag{A.7}$$

$$\Sigma_{\tau}[v] = (i/2) \,\sigma(t) \,v(t). \tag{A.8}$$

The discontinuity in (A.7) and (A.8) is because of the white spectrum for z(t).

A further important process is the generalized Poisson process (shot noise) [11]

$$z(t) = \sum_{k=1}^{n(t)} x_k g(t - t_k),$$
(A.9)

where the random variables x_k are independent of each other and distributed with the probability q(x): n(t) denotes the Poisson counting process with parameter λ . The function g(s) describes the pulse shape and is assumed to satisfy g(s)=0 for s < 0. For this process the characteristic functional has been calculated by Feynman and Hibbs [11] yielding

$$\Phi_t[v] = \exp\left\{\lambda \int_0^t d\tau \left(C\left[\int_{\tau}^t ds \, v(s) \, g(s-\tau)\right] - 1\right)\right\}, \quad (A.10)$$

where

$$C[v] = \int_{-\infty}^{+\infty} dx \, q(x) \exp i x \, v. \tag{A.11}$$

Henceforth, a straightforward calculation gives

$$\Omega_{t,s}[v] = -i\lambda \int_{0}^{s} dr g(s-\tau) \frac{d}{dv} C \left[\int_{\tau}^{t} dr g(r-\tau) v(r) \right]$$

= $\lambda \int_{-\infty}^{+\infty} dx q(x) x \int_{0}^{s} d\tau g(s-\tau)$
 $\cdot \exp \left\{ ix \int_{0}^{t} dr g(r-\tau) v(r) \right\}$ (A.12)

$$\Sigma_t[v] = \Omega_{t,s}[v]|_{s=t}.$$
(A.13)

Thus, the correlation (2.9) becomes

$$\langle z(s) g(z) \rangle = \lambda \int_{-\infty}^{\infty} dx q(x) x \int_{0}^{s} d\tau g(s-\tau)$$

$$\cdot \left\langle \exp\left[x \int_{\tau}^{s} dr g(r-\tau) \frac{\delta}{\delta z(r)}\right] g(z) \right\rangle$$
(A.14)

$$=\lambda \int_{-\infty}^{\infty} dx q(x) x \int_{0}^{s} d\tau g(s-\tau)$$

 $\cdot \langle g[z(r) + x g(r-\tau)] \rangle, \quad 0 \leq s \leq t.$ (A.15)

For a white generalized Poisson process the pulse shape becomes indefinitely sharp $(g(t-s) \rightarrow \delta(t-s))$. Then we obtain from (A.10)

$$\Psi_t[v] = \lambda \int_0^t ds \{ C[v(s)] - 1 \}.$$
 (A.16)

The auxiliary functionals $\Omega_{t,s}$ and Σ_t are calculated to be

Note Added in Proof. After completion of this paper I got aware of the work by V.E. Shapiro and V.M. Loginov, Physica 91 A, 563 (1978): Following a similar reasoning as presented in Section 2, they derive for the special class of processes with an exponential form for the covariance (e.g. the Kubo-Anderson processes) some very useful formulae for correlation functions of the type considered in Equation (2.9).

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$$\Omega_{t,s}[v] = \lambda \int_{-\infty}^{\infty} dx \, q(x) \, x \exp i \, x \, v(s), \tag{A.17}$$

$$\Sigma_t[v] = \lambda \int_{-\infty}^{\infty} dx \, q(x) \int_{0}^{x} du \exp i \, u \, v(t).$$
(A.18)

Due to the discontinuity in the formulas (A.17) and (A.18) we have for the correlation in (A.15) for s=t in this case the expression

$$\langle z(t) g(z) \rangle = \lambda \int_{-\infty}^{\infty} dx q(x) \int_{0}^{x} du \langle g(z(r) + u \,\delta(t - r)) \rangle.$$
(A.19)

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