

# ON THE RELATIONS BETWEEN MARKOVIAN MASTER EQUATIONS AND STOCHASTIC DIFFERENTIAL EQUATIONS<sup>†</sup>

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We have investigated the relationship between Markovian master equations (m.e.) and the corresponding stochastic differential equations (s.d.e.) for closed systems, i.e., systems not subjected to external pumping. We show that the form of the fluctuations in the s.d.e., i.e., additive or multiplicative, depends upon the properties of the kernel of the m.e. and the range of the state space of the stochastic variable(s), i.e., bounded or unbounded. The knowledge of these two properties of the m.e. permits the determination of the way in which the fluctuations enter into the s.d.e. (i.e., additive or multiplicative) and the calculation of their statistics. Several examples are presented to illustrate the general theory.

## 1. Introduction

There has been a significant increase in recent years in the interest in and the study of stochastic differential equations with multiplicative noise. These equations describe (or are supposed to describe) stochastic processes where the fluctuations depend upon values of the system variables. This is in contrast to the more familiar additive noise where the fluctuations do not depend on the values of the system variables. A clear and useful review of such multiplicative stochastic processes has been published recently by Schenzle and Brand<sup>1</sup>).

Two important questions arise in the formulation of stochastic differential equations (s.d.e.) as a phenomenological description of a stochastic process:

(a) In the phenomenological modeling of a stochastic process by a s.d.e., how does one know a priori whether to use additive or multiplicative noise?; and

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(b) In the usual absence of both experimental and basic theoretical information, how does one know (or guess) the specific form of the multiplicative noise?

In the simplest and most studied of stochastic process, i.e., Brownian motion, the answers to these questions are of course known. In the velocity variable formation, the noise is delta-correlated, Gaussian and additive. In the energy variable, it is delta-correlated, Gaussian and multiplicative<sup>2</sup>). In more complicated examples of stochastic processes (chemical kinetics, laser problems, oscillatory systems with fluctuating parameters, population biology, etc.), the answers are not all that clear.

The most fundamental approach to answering the questions posed above would be to start with the Hamiltonian of the systems under study and then derive the s.d.e. via the appropriate Liouville equation. For obvious reasons, we have not chosen this very ambitious path. Our starting point instead is the master equation. For simplicity and to obtain analytic results, we have limited our investigation, for the time being, to Markov master equations. The choice of a starting point has several desirable features: From the work of van Hove, Prigogine, Zwanzig and others<sup>3</sup>) one understands the relation between the Liouville equation and the Markovian master equation. For many physical and chemical processes there exists a simple and quite unequivocal\* methodology for the formulation of phenomenological master equations in the Markovian limit. In some cases it is possible to calculate explicitly the transition rates which enter into the master equation. And finally, and most importantly, the structure of the fluctuations (additive vs. multiplicative, Gaussian vs. non-Gaussian) does not have to be introduced in an a priori explicit manner—it is contained implicitly within the formulation of the master equation.

In this paper we investigate the passage from a Markovian master equation to the corresponding stochastic differential equation. Specifically, we address ourselves to the questions raised above, i.e., what conditions lead to multiplicative noise, what conditions lead to additive noise, and what is the structure of the noise. The general theory developed in Sections 2 through 4 is then applied in section 5 to a number of specific examples.

Our results can be summarized briefly as follows:

(1) Additive noise in stochastic differential equations will be a valid description of fluctuations if and only if the stochastic kernel  $B(x, y)$  of the master equation, as defined in (III. 15), is translationally invariant, i.e., the jump probabilities are functions of the jump distance  $u = x - y$  only.

\* By this we mean that, given a sufficiently well specified physical problem, independent investigators will, with a probability approaching unity, write down identical Markovian master equations.

(a) If the state space of the stochastic variable  $x$  is unbounded, i.e.,  $-\infty \leq x \leq \infty$ , translational invariance implies that  $B(x, y) = B(u)$  is non-negative for both positive and negative  $u$  and may be non-zero (i.e., positive) for both positive and negative  $u$ .

(b) If the state space of the stochastic variable  $x$  is bounded either from above or below by natural boundaries, the kernel  $B(x, y) = B(u)$  must be of a form such that  $B(u) \equiv 0$  for  $u$  positive if  $x$  is bounded from above and  $B(u) \equiv 0$  for  $u$  negative if  $x$  is bounded from below. Such sets of transition probabilities correspond to pure death or birth processes. The additive noise will then be of a form which is bounded from above or below such as the Poisson noise of example 1 in section 5.

(2) Multiplicative noise will be obtained whenever the stochastic kernel  $B(x, y)$  is not translationally invariant, i.e., when the transition probabilities of the master equation are state dependent.

Our results pertain to stochastic systems with "internal" fluctuations, i.e., the dynamics of the systems under study can be naturally described via two widely separated time scales, with the rapid variations of the system variables treated as the fluctuations. We are not considering here systems subjected to "external" noise, i.e., noise which can be arbitrarily initiated and structured by the experimenter.

## 2. Structure of stochastic differential equations for Markovian processes

From a mathematical point of view, there are basically two ways to approach the description of fluctuations in physical systems. The first is the use of master equations; the second is given by Langevin equations. It is only recently that the general relationship between a Langevin description and the corresponding master equation has been investigated<sup>4,5</sup>). In order for the discussions below to be more readily accessible, we reformulate the basis of this relationship in less mathematical terms than in ref. 5. In what follows we outline the theory for stochastic systems described in terms of a finite number of random variables in continuous state space.

We consider a system described by a Markov process  $X(t)$  for which the probability density  $p(x, t)$  obeys the master equation

$$\dot{p}(x, t) = \int \Gamma(x, y)p(y, t) dy. \quad (1)$$

We assume that the transition rate  $\Gamma$  and the probabilities  $p$  are of such a form that one can formally expand the master equation into a Taylor series,

obtaining the (vector) Kramers–Moyal expansion,

$$\dot{p}(\mathbf{x}, t) = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \left[ \frac{\partial}{\partial \mathbf{x}} \right]^{[n]} \Theta \left[ \mathbf{A}_n(\mathbf{x}) p(\mathbf{x}, t) \right], \quad (2)$$

where the notation  $v^{[n]}$  stands for the  $n$ -fold dyadic product of the vector  $v$  and the notation  $\Theta$  stands for the  $n$ -fold contraction. The tensor  $\mathbf{A}_n(\mathbf{x})$  is given by

$$\mathbf{A}_n(\mathbf{x}) = \int (\mathbf{z} - \mathbf{x})^{[n]} \Gamma(\mathbf{z}, \mathbf{x}) d\mathbf{z}. \quad (3)$$

From (2) we postulate that the *mean* evolution of the macrovariables can be described by the truncated equation

$$\frac{\partial}{\partial t} \langle \mathbf{x}(t) \rangle = \langle \mathbf{A}_1(\mathbf{x}(t)) \rangle, \quad (4a)$$

where

$$\langle \mathbf{x}(t) \rangle = \int \mathbf{x} p(\mathbf{x}, t) d\mathbf{x} \quad (4b)$$

and where

$$\langle \mathbf{A}_i(\mathbf{x}(t)) \rangle = \int \mathbf{A}_i(\mathbf{x}) p(\mathbf{x}, t) d\mathbf{x}. \quad (4c)$$

The process  $\mathbf{X}(t)$  can also be formulated in terms of a so-called stochastic differential equation (s.d.e.) or Langevin equation describing directly the sample paths  $\mathbf{x}(t)$  of the process. Such a Langevin equation is then composed of two parts: one part refers to the deterministic evolution, whereas the second part accounts for the fluctuations. There exists no unique prescription for the decomposition of the evolution into a deterministic (drift) and a fluctuating part.

In the following we write a stochastic differential equation which is to be interpreted using Itô calculus. The s.d.e. is

$$\dot{\mathbf{x}}(t) = \mathbf{A}_1(\mathbf{x}(t)) + \boldsymbol{\xi}(t), \quad (5)$$

where  $\boldsymbol{\xi}(t)$  is a stochastic force which may depend on  $\mathbf{x}(t)$ . The average of eq. (5) for fixed value of  $\mathbf{x}(t) = \mathbf{x}$  is

$$\langle \dot{\mathbf{x}}(t) \mid \mathbf{x}(t) = \mathbf{x} \rangle = \mathbf{A}_1(\mathbf{x}) + \langle \boldsymbol{\xi}(t) \mid \mathbf{x}(t) = \mathbf{x} \rangle. \quad (6)$$

We now use the Itô prescription

$$\langle \boldsymbol{\xi}(t) \mid \mathbf{x}(t) = \mathbf{x} \rangle = 0 \quad (7)$$

for all  $x$  and eq. (6) then becomes

$$\langle \dot{x}(t) \mid x(t) = x \rangle = A_1(x). \tag{8}$$

When eq. (8) is averaged over all values of  $x(t)$  consistent with the initial conditions, i.e., over all stochastic realizations, we obtain eq. (4a).

The s.d.e., eq. (5), represents a Markov process if and only if the stochastic forces,  $\xi(t)$ , have delta-correlated cumulants of all order. Eq. (5) is an equivalent representation of the Markov process  $x(t)$  described by the master equation in (4) with the Kramers–Moyal moments given in (2), if, for given  $x(t) \equiv x$ , the random force cumulants have the property<sup>5)</sup>:

$$\begin{aligned} \lim_{\Delta \rightarrow 0} \frac{1}{\Delta} \int_t^{t+\Delta} dt_1 \int_t^{t+\Delta} dt_2 \cdots \int_t^{t+\Delta} dt_n \langle \xi(t_1) \cdots \xi(t_n) \mid x(t) = x \rangle_c \\ = A_n(x), \quad n \geq 2, \end{aligned} \tag{9a}$$

which is equivalent to

$$\langle \xi(t_1) \cdots \xi(t_n) \mid x(t) = x \rangle_c = A_n(x) \delta(t_1 - t_2) \cdots \delta(t_{n-1} - t_n), \quad n \geq 2 \tag{9b}$$

where  $t + \Delta \geq t_1, \dots, t_n \geq t$ . Here the subscript  $c$  denotes the cumulant average and the average is taken for fixed  $x(t)$ .

The white noise source  $\xi(t)$  in (8) can be decomposed into a part composed of delta-correlated Gaussian noise  $\eta_G(t)$  describing the continuous displacement of a sample path and a part composed of delta-correlated Poisson noise  $\eta_p(t, du)$  of vanishing mean describing discontinuous jumps of length between  $(u, u + du)$ . In this context a possible delta-correlated Gaussian component can be looked upon as the limit of a symmetric jump process with jump frequency  $\nu \rightarrow \infty$  and jump length  $u \rightarrow 0$  such that  $\nu u^2$  remains finite<sup>6)</sup>. In terms of the components  $\eta_G(t)$  and  $\eta_p(t, du)$ , the delta-correlated noise  $\xi(t)$  has the linear functional representation<sup>7)</sup>

$$\xi(t) = g(t)\eta_G(t) + \int f(t, u)\eta_p(t, du), \tag{10}$$

where the functions  $g(t)$  and  $f(t, u)$  are determined by the physics of the problem. Here  $\eta_G(t)$  denotes a vector of independent Gaussian delta-correlated processes  $\eta_G^{(i)}(t)$ ,  $i = 1, \dots$ .

In what follows, we call the noise  $\xi(t)$  *multiplicative* noise if at least one of the cumulant averages in (9) for  $n \geq 2$  is explicitly  $x$ -dependent, that is, if at least one Kramers–Moyal moment  $A_n(x)$  for  $n \geq 2$  becomes a function of  $x$ . As a consequence, the functions  $g(t)$  or  $f(t, u)$  are necessarily non-constant functions of  $x$ . On the other hand, if  $A_n$  is constant for all  $n \geq 2$ , then the

functions of  $g$ ,  $f$  and  $\xi$  become independent of  $x$  and one obtains additive noise.

### 3 Markovian processes with additive noise

In this section we will discuss the relation between the master equation and stochastic differential equations with additive noise. Throughout this section it is assumed that the stochastic variables  $x$  are defined on the *unrestricted* real space. Given a specific master equation, the previous discussion shows that the necessary and sufficient condition for additive noise reads

$$\mathbf{A}_n \equiv \int (x - y)^{[n]} \Gamma(x, y) dx = \text{independent of } x, \quad (11)$$

for all  $n \geq 2$ . As a consequence, i.e., in order for (11) to hold for  $n \geq 2$ , the kernel  $\Gamma(x, y)$  must be of the form

$$\Gamma(x, y) = A_1(y) \delta'(y - x) + K(x - y). \quad (12)$$

For  $(x - y) = u$ , eq. (11) can be rewritten as

$$\mathbf{A}_n = \int u^{[n]} K(u) du, \quad n \geq 2. \quad (13)$$

Note that in order for eq. (11) to yield the correct expression for  $A_1$  with the kernel  $\Gamma(x, y)$  given in eq. (12), the kernel  $K$  must be of a form such that

$$\int (x - y) K(x - y) dx = 0. \quad (14)$$

For the kernel  $K(u)$  defined in eq. (12), we can write

$$\mathbf{K}(u) = \mathbf{B}(u) - \gamma \delta(u) \quad (15)$$

where  $\gamma$  is the total jump frequency, i.e.,

$$\gamma = \int \mathbf{B}(u) du. \quad (16)$$

Using eqs. (15) and (16), we can now rewrite the master equation (1) with the kernel  $\Gamma(x, y)$  given in eq. (12) in the usual "gain-loss" form as

$$\dot{p}(x, t) = -\frac{\partial}{\partial x} A_1(x) p(x, t) + \int B(x - y) p(y, t) dy - \gamma p(x, t). \quad (17)$$

The stochastic differential equation (s.d.e.) for the master equation (17) can

now be written as

$$\dot{x}(t) = A_1(x(t)) + \xi(t), \tag{18}$$

where from eq. (9) the *additive* noise  $\xi(t)$  has the conditional cumulants

$$\langle \xi(t_1) \cdots \xi(t_n) | x(t) = x \rangle_c = \left( \int u^{[n]} B(u) du \right)^n \times \delta(t_1 - t_2) \cdots \delta(t_{n-1} - t_n), \quad n \geq 2. \tag{19}$$

The Kramers–Moyal moments  $A_n$  of eq. (11) are thus given by

$$A_n = \int u^{[n]} B(u) du, \quad n \geq 2, \tag{20}$$

consistent with (13).

By use of the properties of white Poisson noise<sup>5)</sup> we find further for  $\xi(t)$  from (19) the explicit representation [see eq. (10)]

$$\xi(t) = g\eta_G(t) + \int u\eta_p(t, du). \tag{21}$$

The results of eq. (17) and the corresponding s.d.e. (18) with the noise given by eqs (19) and (21) are one of the principal results of this paper. *Additive noise in the stochastic differential equation formulation will be obtained if and only if the corresponding master equation has a kernel  $K(x, y)$ , which is a function only of the jump distance  $u = x - y$ .* Conversely, any stochastic process whose transition probabilities are state dependent, i.e., the kernel  $K(x, y)$  is an explicit function of  $x$  (or  $y$ ) in addition to  $(x - y)$ , cannot be formulated by a stochastic differential equation with additive noise\*.

The above discussion shows that the phenomenological modeling of a statistical system in terms of additive noise is certainly limited. For a physical system whose bare dissipative transport coefficients are given by the Kramers–Moyal moments  $A_n(x)$  with  $n \geq 2$ , the generally non-linear dependence of the transport coefficients on the state variables must be small as measured by some dimensionless expansion parameter for modeling in terms of additive noise to be approximately valid. In this context, it is presently very popular to model phenomenologically the order parameter in a dynamical system by a time-dependent stochastic equation of the Ginzburg–Landau

\*It should be noted that additive noise is not a covariant property. Any *non-linear*, time-independent change of representation of the type  $x \rightarrow x' = g(x)$  will transform the additive noise  $\xi(t)$  into a multiplicative noise. Conversely, for a system with multiplicative noise there may exist a non-linear inverse transformation which changes multiplicative noise into an additive one<sup>8,9)</sup>. Such a transformation, for example, *always* exists in the case of a s.d.e. in one dimension<sup>2,8)</sup>.

type<sup>10</sup>) in which the noise  $\xi(t)$  is usually assumed to be additive delta-correlated Gaussian noise. The strength of the noise is usually fixed via a fluctuation-dissipation theorem (of the second kind) which relates the linear dissipative transport coefficient with the correlation of the noise. We would like to remark that the application of this approach is generally limited; it is based on a priori specification of the noise structure whose (approximate) validity should be checked independently. Moreover, knowledge of the deterministic dynamical equations is not sufficient to fix the noise structure uniquely<sup>11</sup>).

However, although the stochastics of the system dynamics is generally non-linear in the sense of multiplicative noise, this might show up only in the form of nonlinear dissipative transport laws, whereas the behavior of small fluctuations about the average behavior may be quasi-linear<sup>8,12-14</sup>). An important result in this context is the work of Grabert<sup>12</sup>). Starting from non-linear macroscopic transport laws, he was able to derive a *linear* generalized Langevin equation for the fluctuations of the macrovariables around the time-dependent mean-value behavior. In the Markov limit, this equation will, under certain conditions<sup>8</sup>), reduce to a Gaussian-Markovian process with renormalized transport coefficients, thus providing a statistical foundation of the phenomenological approaches developed by Van Kampen<sup>13</sup>) and Kubo et al.<sup>14</sup>). Such an approach can be looked upon as one in which the effect of multiplicative noise is incorporated into the renormalized non-linear mean-value equations.

#### 4. Stochastic processes in restricted state space

Stochastic processes on a restricted state space are basically of two types: (a) those with natural boundary conditions (i.e., the master equation as written is valid for *all* values of the state variable within the restricted space); and (b) those where boundary conditions must be explicitly supplied (i.e., the master equation for the process is not valid for all values of the state variable and a separate equation(s) must be written for the state variables at or near the boundaries). For processes described by master equations of type (b), such as Brownian motion in coordinate space with a reflecting boundary at  $x = 0$ , we do not presently see how to construct the equivalent stochastic differential equation. *In what follows, we restrict ourselves to processes of type (a).*

The important point to realize for stochastic processes on a restricted state space is that the fluctuation in the s.d.e. must not drive the system beyond the boundaries. For processes of type (a) above, one has to distinguish between two cases: (i) pure birth or death processes and (ii) processes with both positive and negative transitions. For case (i), it is possible, as we shall show

in the next section, to have purely additive noise if such noise is properly bounded from below or above. An example of this type of behavior is furnished by a birth or death process with constant transition probabilities which leads to properly bounded additive Poisson noise. On the other hand, as we shall also show in the next section, pure birth or death processes with state dependent transition probabilities will lead to multiplicative noise. For case (ii), natural boundary conditions will obtain only for master equations with state dependent transition probabilities. This implies that the corresponding s.d.e. will necessarily have multiplicative noise. Thus, for instance, the s.d.e. for a quantum system described by a Pauli-type master equation must necessarily have multiplicative noise since (a) the quantum states, characterized by their quantum numbers, are bounded from below and (b) the requirement of detailed balancing for such systems leads to state dependent transition probabilities. This multiplicative noise structure for the s.d.e. will also necessarily obtain for all "gain-loss" stochastic descriptions of rate processes in particle number space since the state space for such systems is obviously bounded from below at a (particle number) = 0. The next section contains some examples of such systems which demonstrate the points made above.

A word of caution is in order here about the relation between master equations (whether in discrete or continuous state space) with natural boundary conditions and the Fokker-Planck equation obtained via Kramers-Moyal expansions which are supposed to be approximations to such master equations. Care must be taken in the criteria used in terminating the K-M expansion with  $A_2(x)$  in that these criteria must result in a Fokker-Planck equation with corresponding natural boundary conditions. Thus, for instance, if there is a reflecting boundary at  $x = 0$ , it is necessary that  $A_2(x)$  be of such a form that  $A_2(x = 0) = 0$ . We return to this point in some of the examples of the next section.

## 5. Examples

As our first example we study a Poisson process  $N(t) \geq 0$  with jump length  $u = 1$ . Specifically, we will investigate the connection between the master equation and the corresponding s.d.e. for radioactive decay. Let  $P(N, t)$  be the probability that  $N$   $\alpha$ -particles have been emitted from the nuclei in the time interval  $(0, t)$ . The master equation governing this process is<sup>15)</sup>

$$\dot{P}(N, t) = \lambda[P(N-1, t) - P(N, t)], \quad N = 1, 2, \dots, \quad (22)$$

$$\dot{P}(0, t) = -\lambda P(0, t), \quad N = 0, \quad (23)$$

with the initial condition  $P(N, 0) = \delta_{N,0}$ . This is a pure "birth" process with the constant transition rate  $\Gamma = \text{constant} = \lambda$ . The solution to eqs. (22) and (23) is the Poisson distribution

$$P(N, t) = \frac{(\lambda t)^N}{N!} e^{-\lambda t} \quad (24)$$

to which we make reference again below.

Writing the probability  $P(N, t)$  in terms of the probability density  $p(x, t)$  as

$$P(N, t) = \int_{N-1/2}^{N+1/2} p(x, t) dx, \quad (25)$$

we can write the master equation for  $p(x, t)$  as

$$\begin{aligned} \dot{p}(x, t) &= \lambda \left[ \int \delta(x - y - 1) p(y, t) dy - p(x, t) \right] \\ &= -\lambda \frac{\partial}{\partial x} p(x, t) + \lambda \sum_{n=2}^{\infty} \frac{(-1)^n}{n!} \frac{\partial^n p(x, t)}{\partial x^n}. \end{aligned} \quad (26)$$

Note that the Kramers–Moyal expansion of a discrete master equation must be handled with great care. This is particularly true if the discrete variable cannot take on all discrete values between  $-\infty$  and  $+\infty$ . For a discussion of these points, see ref. 16. In our development, we shall use eq. (26) only to obtain the s.d.e.

The Kramers–Moyal moments  $A_n$  are thus constant,

$$A_n = \lambda, \quad n \geq 1, \quad (27)$$

and the corresponding s.d.e. can be written as

$$\dot{x} = \lambda + \xi(t, u = 1) = \lambda + \eta_p(t, u = 1), \quad (28)$$

with initial condition  $x(0) = 0$ . The noise  $\xi(t, u = 1)$  is a delta-correlated, additive Poisson noise satisfying

$$\langle \xi(t) \rangle = 0, \quad (29)$$

$$\langle \xi(t_1) \cdots \xi(t_n) \rangle_c = \lambda \delta(t_1 - t_2) \cdots \delta(t_{n-1} - t_n), \quad n \geq 2, \quad (30)$$

$$\xi(t, u = 1) = \sum_i \delta(t - t_i) - \lambda, \quad (31)$$

with  $t_i$  a Poisson arrival time. The realizations of the Poisson noise  $\xi(t)$  are thus bounded from below at  $-\lambda$ .

We are dealing here with the restricted state space  $0 \leq N \leq N_0$ , where  $N_0$  is the number of  $\alpha$ -particles emitted in the time interval  $(0, \infty)$ , i.e.,  $N_0$  is the

initial number of  $\alpha$  particles in the nuclei. As we will show below, eq. (22) is a valid representation of radioactive decay only in the limits  $N_0$  is sufficiently large and that the total time-interval  $(0, t)$  of data acquisition is sufficiently short such that  $N_0 - N \approx N_0$ . Under these conditions, it is clear from the structure of the s.d.e. (28) and the lower bound on  $\xi(t)$  that the additive Poisson noise cannot drive the state variable  $x$  outside the boundaries  $(0, N_0 \rightarrow \infty)$  of the state space.

For our next example, we consider the first order chemical reaction  $B \xrightarrow{\lambda} C$  where a substance  $B$  is converted to  $C$  with a rate coefficient  $\lambda$  without back reaction. If we let  $\mathcal{P}(N, t)$  be the probability that  $N$  molecules of species  $B$  are present at time  $t$ , the master equation for this reaction can be written as<sup>15)</sup>

$$\dot{\mathcal{P}}(N, t) = \lambda[(N + 1)\mathcal{P}(N + 1, t) - N\mathcal{P}(N, T)], \quad N = 0, 1 \dots, \quad (32)$$

with the initial condition  $\mathcal{P}(N, 0) = \delta_{N, N_0}$ . This is a pure death process with natural boundary conditions and state dependent transition probabilities. Proceeding by the methods discussed in sections 2 and 3, one can readily find, using the definition of  $p(x, t)$  in eq. (25), that the s.d.e. corresponding to the master equation (32) is

$$\dot{x}(t) = -\lambda x(t) + \xi(t), \quad (33)$$

with  $x(0) = N_0$ , i.e., we now obtain multiplicative noise as expected. The delta-correlated noise  $\xi(t)$  obeys the statistical properties

$$\langle \xi(t) \mid x(t) = x \rangle = 0, \quad (34a)$$

$$\langle [\xi(x(t_1)) \cdots \xi(x(t_n))] \mid x(t) = x \rangle_c = (-1)^n \lambda x \delta(t_1 - t_2) \cdots \delta(t_{n-1} - t_n),$$

$$t + \Delta \geq t_1, \dots, t_n \geq t. \quad (34b)$$

We are dealing here with a restricted state space  $0 \leq N \leq N_0$ . Since  $N$  is bounded from below at  $N = 0$ , the noise must not drive  $N$  below  $N = 0$ . This is explicitly taken care of by the multiplicative nature of the noise, which is of the form that  $\xi(t) \rightarrow 0$  as  $x \rightarrow 0$ . Van Kampen<sup>17)</sup> has treated this problem using different techniques but our results are equivalent.

It should be noted that eq. (32) can also be interpreted as the master equation for radioactive decay if we define  $\mathcal{P}(N, t)$  as the probability that there are  $N$   $\alpha$ -particles (radioactive nuclei) remaining at time  $t$  if there were  $N_0$  at time  $t = 0$ . The solution of eq. (32) subject to the initial condition  $\mathcal{P}(N, 0) = \delta_{N, N_0}$  is<sup>15)</sup>

$$\mathcal{P}(N, t) = \binom{N_0}{N} (1 - e^{-\lambda t})^{N_0 - N} e^{-N\lambda t}, \quad (35)$$

i.e.,  $\mathcal{P}(N, t)$  is a binomial distribution. The relationship between  $P(N, t)$  and  $\mathcal{P}(N, t)$  is  $\mathcal{P}(N, t) = P(N_0 - N, t)$ . In the limits  $N_0 \rightarrow \infty$ ,  $\lambda t \rightarrow 0$  such that  $N_0 \lambda t$  is finite and  $N_0 \approx N$ , this binomial distribution converges to a Poisson distribution. In this limit, eq. (32) gives rise to a stochastic differential equation analogous to that in eq. (28) with additive, delta-correlated Poisson noise. It should also be noted that in the limit  $N \rightarrow \infty$ , the state variable  $N$  is essentially constant over some sufficiently short time interval  $(0, t)$ . For this case the factor  $\lambda N (= \lambda x)$  in front of the delta function product of eq. (34b) can be replaced by a constant transition rate  $\lambda'$ . As discussed above, the master equation (22) for radioactive decay which leads to additive Poisson noise is thus valid only (a) for a very large initial concentration  $N_0$  of radioactive atoms and (b) for a sufficiently short time interval  $(0, t)$ .

For our next example, we consider the Montroll-Rubin-Shuler model of the vibrational relaxation of identical harmonic oscillators in interaction with a heat bath<sup>18,19</sup>. The master equation for the transitions between different vibrational energy levels  $N = 0, 1, \dots$  of the oscillator can be described as a birth and death process with the state dependent transition rates<sup>18,19</sup>

$$\Gamma^+(N \rightarrow N + 1) = \kappa(N + 1)e^{-\theta}, \quad \theta = h\nu/k_B T, \quad (36)$$

$$\Gamma^-(N \rightarrow N - 1) = \kappa N, \quad (37)$$

where  $\kappa$  is the coupling constant between the oscillator molecules and the heat bath. For  $\theta \ll 1$ , i.e., for sufficiently small energy level spacing  $h\nu$  or at sufficiently high temperature  $T$ , the above master equation can be approximated by the Fokker-Planck equation<sup>18</sup>

$$P(N, t) = \int_{N-1/2}^{N+1/2} p(x, t) dx, \quad (38)$$

$$\dot{p}(x, t) = \kappa \frac{\partial}{\partial x} \left[ x e^{-\theta x} \frac{\partial}{\partial x} e^{\theta x} p(x, t) \right]. \quad (39)$$

In terms of the dimensionless time  $\tau = \kappa y$ , eq. (39) can be recast in the more familiar form

$$\dot{p}(x, \tau) = -\frac{\partial}{\partial x} [(1 - \theta x)p(x, \tau)] + \frac{\partial^2}{\partial x^2} [xp(x, \tau)]. \quad (40)$$

The master equation with the transition probabilities (36) and (37) has natural boundary conditions [ $\Gamma^+(-1 \rightarrow 0) = 0$ ,  $\Gamma^-(0 \rightarrow -1) = 0$ ] which are preserved in the Fokker-Planck approximation (40). This is expressed therein by the vanishing of the diffusion current at  $x = 0$ . The Itô-s.d.e. corresponding to the

Fokker-Planck eq. (40) is

$$\dot{x}(t) = [1 - \theta x(t)] + \sqrt{2x(t)} \eta_G(t). \tag{41}$$

where  $\eta_G(t)$  is the delta-correlated Gaussian noise of eq. (10). The form of the multiplicative noise insures that the fluctuations cannot drive the state variable  $x$  below its lower bound at  $x = 0$  since the fluctuations go to zero as  $x \rightarrow 0$ .

As a final example, we consider the three-dimensional Rayleigh gas problem<sup>20-22</sup>). It describes the dynamics of a dilute ensemble of heavy particles (mass  $m_1$ ) which undergoes collisions with light heat bath particles of mass  $m_2 \leq m_1$ , which maintain a Maxwellian equilibrium distribution at temperature  $T$ . Using the reduced kinetic energy  $x = m_1 v^2 / kT$  as the stochastic variable (which is bounded from below at  $x = 0$ ), the master equation for  $p(x, t)$  reads

$$\dot{p}(x, t) = \int w(x, y) p(y, t) dy - \lambda(x) p(x, t), \tag{42}$$

where the stochastic kernel  $w(x, y)$  is given by<sup>21</sup>)

$$w(x, y) = \frac{1}{2} Z Q^2 \frac{\pi^{1/2}}{y^2} \left\{ \text{erf}(Qx^{1/2} + Ry^{1/2}) + e^{y-x} \text{erf}(Rx^{1/2} + Qy^{1/2}) \right. \\ \left. \pm [\text{erf}(Qx^{1/2} - Ry^{1/2}) + e^{y-x} \text{erf}(Rx^{1/2} - Qy^{1/2})] \right\}. \tag{43}$$

(+ for  $x < y$ ; - for  $x > y$ ).

The master equation (42) with the kernel (43) has natural boundary conditions at  $x = 0$ . The quantity  $Z$  is a collision number and  $Q$  and  $R$  are related to the mass ratio of  $\gamma = m_2 / m_1 < 1$  by

$$Q = \frac{1}{2}(\gamma^{-1/2} + \gamma^{1/2}); \quad R = \frac{1}{2}(\gamma^{-1/2} - \gamma^{1/2}). \tag{44}$$

The notation  $\text{erf}(x)$  denotes the usual error function

$$\text{erf } x = \frac{2}{\pi^{1/2}} \int_0^x e^{-s^2} ds. \tag{45}$$

The energy dependent total jump frequency  $\lambda(x)$  can be calculated from (43) to be

$$\lambda(x) = Z \gamma^{-1/2} \left[ \left( 2(\gamma x)^{1/2} + (\gamma x)^{-1/2} \frac{\pi^{1/2}}{2} \text{erf}(\gamma x)^{1/2} + e^{-\gamma x} \right) \right]. \tag{46}$$

The Kramers-Moyal moments  $A_n(x)$ ,

$$A_n(x) = \int_0^\infty (y - x)^n w(y, x) dy, \quad n \geq 1, \tag{47}$$

have been calculated by Andersen and Shuler<sup>21)</sup> to give

$$A_n(x) = \frac{ZQ^2\pi^{1/2}}{x^{1/2}} I_n(x). \quad (48)$$

The function  $I_n(x)$  has a rather complicated structure<sup>21)</sup> which will not be reproduced here owing to its excessive length. The first moment  $A_1(x)$  giving the "bare" drift is

$$\begin{aligned} A_1(x) &= \frac{Z\pi^{1/2}}{2Q^2} \left\{ \left[ -x^2 + \left(2 - \frac{1}{\gamma}\right)x + \frac{1}{\gamma} \left(1 + \frac{1}{4\gamma}\right) \right] \frac{\text{erf}(\gamma x)^{1/2}}{x^{1/2}} \right. \\ &\quad \left. + \gamma^{-1/2} \left( -\frac{1}{2}x + 1 - \frac{1}{4\gamma} \right) \exp(-\gamma x) \right\} \\ &= \frac{8}{3}\gamma \left( \frac{3}{2} - x \right) \lambda(x) + \mathcal{O}(\gamma x) \end{aligned} \quad (49)$$

and the second moment is given by

$$A_2(x) = \frac{16}{3}\gamma x \lambda(x) + \mathcal{O}(\gamma x). \quad (50)$$

The higher moments  $A_n(x)$  are small compared with  $A_1(x)$ ,  $A_2(x)$ , with

$$A_n(x)/A_1(x), A_n(x)/A_2(x) = \mathcal{O}(\gamma x) \text{ or higher for } n \geq 3. \quad (51)$$

From (48) it follows that the master equation (42) with the kernel (43) is equivalent to an Itô-s.d.e. of the form of eq. (8), i.e.,

$$\dot{x}(t) = A_1(x(t)) + \xi(t), \quad (52)$$

with  $A_1(x)$  given by eq. (49) and  $\xi(t)$  a multiplicative, delta-correlated noise satisfying the relation (9) with  $A_n(x)$  given by (48). It is clear that in this general formulation the noise has a very complicated structure. A great simplification can be achieved for  $\gamma \equiv m_2/m_1 \ll 1$  which corresponds to the Brownian motion limit of very heavy subsystem particles in a heat bath of very light particles. Using eqs. (49), (50), and (51) and introducing the scaled time  $\tau = 8/3\gamma\lambda(x)t$ , one can rewrite the s.d.e. of eq. (52) as

$$\dot{x}(\tau) = \left( \frac{3}{2} - x(\tau) \right) + \sqrt{2x(\tau)} \eta_G(\tau), \quad (53)$$

where  $\eta_G$  is the delta-correlated Gaussian noise defined in eq. (10). The corresponding Fokker-Planck equation is

$$\dot{p}(x, \tau) = -\frac{\partial}{\partial x} \left[ \left( \frac{3}{2} - x \right) p(x, \tau) \right] + \frac{\partial^2}{\partial x^2} [x p(x, \tau)]$$

in agreement with the results of Andersen and Shuler<sup>21)</sup>.

It should be noted that the last two examples considered here, namely the

vibrational relaxation of harmonic oscillators in the limit  $\theta \ll 1$  and the relaxation of heavy particles in a heat bath of light particles in the limit  $\gamma \ll 1$ , are particular cases of Brownian motion in the continuous energy space  $x$  bounded from below at  $x = 0$ . Comparison of the s.d.e.'s (41) and (53) show that they have identical structure. The noise terms are identical and the drift terms are both linear in  $x$  although of somewhat different form reflecting the different "physics" of these two problems. Equations (41) and (53) are also of the same form as the s.d.e. for the Brownian motion in energy space obtained in ref. 2.

Hoare<sup>22)</sup> has studied the Rayleigh gas in velocity space  $-\infty \leq v \leq \infty$  and has derived the stochastic kernel  $w(v, v')$  corresponding to our expression (43). In the Brownian motion limit  $\gamma \ll 1$  his master equation goes over to the usual Langevin equation in velocity space with *additive noise* since (a) the state space is now unbounded ( $-\infty < v < \infty$ ) and (b) his kernel  $w(v, v')$  is, in the limit  $\gamma \ll 1$ , translationally invariant, being a function of  $(v - v')$  only.

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