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Gaussian white noise as a many-particle process: the Kardar–Parisi–Zhang equation

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Abstract. A new approach is proposed to derive a stochastic differential equation from a Master equation. Starting from the Liouvillian in a Fock space formulation and using a functional integral representation in terms of coherent states we get the corresponding Langevin equation. As examples aggregation and segregation processes with different probability rates are analysed. In the case of a state dependent growth rate it results in a generalized Kardar–Parisi–Zhang equation [7] including the kind of noise which is a purely Gaussian one in this model.

There are different levels to study mesoscopic systems including fluctuations [1, 2]. Langevin's theory of Brownian motion became the prototype for many other models. The separation of time scales has to be regarded as an essential assumption in such an approach. The slowly changing degrees of freedom are considered disconnected from the rapid changing ones. This procedure leads simply to a differential equation with an additive coupling of the deterministic and the stochastic parts. However, the kind of stochasticity included in the equation is to be considered as an input for the model. On the mesoscopic level of description it cannot be deduced from more general principles. In most situations a simple Gaussian distribution is applied, above all because of its simplicity.

Hence, it seems to be necessary to establish a more microscopic approach in which all degrees of freedom are included without a timescale separation from the beginning. With other words every considered degree of freedom should contribute as well as too the deterministic as to the stochastic part of the corresponding dynamic equation. Therefore it is the aim of this paper to propose a consistent and closed scheme to elucidate the structure of the stochastic differential equation starting from a more microscopic approach based on a Master equation (see equation (1)) which can be derived under very general conditions characteristic for Markov processes [1, 2]. In our approach the transition probabilities occurring in the Master equation will be specified in accordance with the physical situation. As an example we will discuss the aggregation process in the reaction limited growth regime [6, 7].

The usual way deriving stochastic differential equations consists in an approximative treatment of Master equations in the limit of small transfer i.e. the transition probabilities are assumed to be negligible for large changes in the considered variables. In this case one can derive via a Kramers–Moyal expansion or van Kampen's expansion [1, 2] a Fokker–Planck type equation which will be reduced to the ordinary Fokker–Planck equation (FP) if only second order moments of the transition probability are taken into account. The FP is equivalent to a Langevin equation.

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Here we proceed in another direction. We start from a Master equation written in terms of creation and annihilation operators in a Fock space representation introduced by Doi [3] and further developed in [4] and [5]. The advantage of this procedure is to give a closed scheme for finding out kinetic equations demonstrated recently [6] in a fermionic approach. However, there has been no derivation of explicit noise terms up to now.

Here we use the bosonic formalism in terms of coherent states which allows to derive stochastic differential equations for certain processes. From the beginning all degrees of freedom will be considered likewise. The separation into different time scales is only determined through the probabilities by which elementary microscopic processes are realized. For special applications we need only the assumption that the creation of an additional particle does not change the state of the system decisively provided there is a large number of particles available. The mathematical formulation of this approximation is given later in (13).

The paper is organized as follows. First we briefly discuss the Fock space formalism for bosonic systems. Further the functional integral representation for the states of the system is established where we follow [5] in a slightly modified form. As a simple example we consider aggregation and segregation of particles on a lattice with different but constant probabilities per time interval. In this case we get a stochastic differential equation. A more complicated example is the aggregation process with a growth velocity dependent locally on the considered state and its neighbouring ones. There results a stochastic differential equation for a growing interface which reduces in the limit of small gradients ((see equation (24)) to the Kardar–Parisi–Zhang equation (KPZ).

The quantities of interest are occupation numbers $\boldsymbol{n}=\{n_i\}$ on a d-dimensional lattice, where i is the number of a lattice site. Our approach is based on a Master equation for the probabilities $F(\boldsymbol{n}, t)$

$$\partial_t F(\boldsymbol{n}, t) = L' F(\boldsymbol{n}, t) \tag{1}$$

L' is an appropriate linear operator specified for the examples investigated below.

According to [3–5] the probabilities $F(\boldsymbol{n}, t)$ and the operator L' are mapped into a Hilbert-space:

$$F(n, t) \Rightarrow |F(t)\rangle$$

$$L' \Rightarrow L.$$

The rate equation (1) corresponds to an equation in the Hilbert-space

$$\partial_t |F((t)\rangle = L|F(t)\rangle \tag{2}$$

which has to be solved.

A complete basis $|\boldsymbol{n}\rangle$ with a scalar product $\langle \boldsymbol{n}|\boldsymbol{m}\rangle = \Pi_i \{n_i! \delta_{m_i,n_i}\}$ is introduced [4, 5] with

$$|F(t)\rangle = \sum_{\boldsymbol{n}} F(\boldsymbol{n}, t)|\boldsymbol{n}\rangle. \tag{3}$$

Creation and annihilation operators are defined [4, 5] as well as the inverse of the creation operators which prove to be useful for the models discussed below.

$$c_i^+ |\ldots n_i \ldots\rangle = |\ldots n_i + 1 \ldots\rangle \tag{4a}$$

$$c_i |\ldots n_i \ldots\rangle = n_i |\ldots n_i - 1 \ldots\rangle \tag{4b}$$

$$(c_i^+)^{-1} |\ldots n_i + 1 \ldots\rangle = |\ldots n_i \ldots\rangle. \tag{4c}$$

Since there is no restriction to the occupation numbers the creation and annihilation operators obey bosonic commutation relations.

The average of a physical quantity $B(\boldsymbol{n})$ is given by [3–5]:

$$\langle B(t)\rangle = \sum_{\{n_i\}} F(\boldsymbol{n}, t) B(\boldsymbol{n}) = \langle s|B|F(t)\rangle \tag{5}$$

with $\langle s| = \langle 0|\, \mathrm{e}^{\Sigma_i c_i}$ and $\langle s|F(t)\rangle = 1$.

A simple relation for the dynamics of averaged quantities follows from equations (2) and (5):

$$\partial_t \langle B(t)\rangle = \langle s|BL|F(t)\rangle. \tag{6}$$

Next we define coherent states as the eigenstates of the creation operators. They are given by:

$$|\boldsymbol{\alpha}\rangle = \mathrm{e}^{\alpha c^+}|0\rangle. \tag{7}$$

Here, the α_i are complex numbers. For real α_i we define normalized coherent states as $|\boldsymbol{\alpha}\rangle_N = \mathrm{e}^{-\Sigma_i \alpha_i}|\boldsymbol{\alpha}\rangle$ which correspond to a Poisson distribution for the n_i with average values α_i.

Using the completeness of the coherent states we find for the solution of equation (2) a path integral representation (compare [5]).

$$|F(t)\rangle = \int \prod_i [d\pi_i(\tau) d\alpha_i(\tau)]\, \mathrm{e}^{-S[\boldsymbol{\alpha}(\tau), \boldsymbol{\pi}(\tau)] + \Sigma_i (\alpha_i(t) - \alpha_i(0))} |\boldsymbol{\alpha}(t)\rangle_N$$

$$\text{with} \quad |F(0)\rangle = |\boldsymbol{\alpha}(0)\rangle_N \tag{8}$$

and

$$S[\boldsymbol{\alpha}(\tau), \boldsymbol{\pi}(\tau)] = \int_0^t d\tau \{ i\boldsymbol{\pi}(\tau) \partial_\tau \boldsymbol{\alpha}(\tau) - \langle -i\boldsymbol{\pi}(\tau)|L|\boldsymbol{\alpha}(\tau)\rangle_N \}.$$

Here $\langle \boldsymbol{\gamma}|L|\boldsymbol{\beta}\rangle_N = \langle \boldsymbol{\gamma}|L|\boldsymbol{\beta}\rangle \langle \boldsymbol{\gamma}|\boldsymbol{\beta}\rangle^{-1}$ are normalized matrix elements. For simplicity we have assumed the system to be in a normalized coherent state at the beginning.

Writing equation (8) as

$$|F(t)\rangle = \int \prod_i [d\alpha_i] F_\alpha(\boldsymbol{\alpha}, t) |\boldsymbol{\alpha}\rangle_N \tag{9}$$

we get the probability to find the system in a normalized coherent state $|\boldsymbol{\alpha}\rangle_N$ at time t:

$$F_\alpha(\boldsymbol{\alpha}, t) = \int_{|\boldsymbol{\alpha}(0)\rangle_N = |F(0)\rangle}^{\boldsymbol{\alpha}(t) = \boldsymbol{\alpha}} \prod_i [d\pi_i(\tau) d\alpha_i(\tau)]\, \mathrm{e}^{-S[\boldsymbol{\alpha}(\tau), \boldsymbol{\pi}(\tau)] + \Sigma_i [\alpha_i(t) - \alpha_i(0)]}. \tag{10}$$

Equations (2), (5) and (10) provide a general tool for treating various problems as diffusion, chemical reaction or aggregation processes.

Next we consider a simple model for deposition of particles on a lattice. Particles are deposited with probability $(v + \sigma^2/2)dt$ and removed from the lattice with probability $\sigma^2 dt/2$ during dt. v and σ^2 are constant rates and $v > 0$. The evolution of the system is described by equation (2) with the Liouvillian:

$$L_G = \sum_i \left\{ v[c_i^+ - 1] + \frac{\sigma^2}{2} [c_i^+ + (c_i^+)^{-1} - 2] \right\}. \tag{11}$$

Using equation (5) and the commutation relations for the operators we get for the occupation numbers:

$$\langle n_i(t)\rangle = \langle n_i(0)\rangle + vt \tag{12a}$$

$$\langle (n_i(t) - \langle n_i(t)\rangle)^2\rangle = (\sigma^2 + v)t. \tag{12b}$$

Expressions of this kind are well known from processes with Gaussian white noise.

We will derive a stochastic differential equation for the occupation numbers. For this reason we write:

$$c_i^+ |F(t)\rangle = |F(t)\rangle \tag{13}$$

which is approximately fulfilled if the system starts from a coherent or deterministic state with $\langle n(0)\rangle \gg 1$. Using equation (13) the Liouvillian can be written as:

$$L_G = \sum_i \left\{ v[c_i^+ - 1] + \frac{\sigma^2}{2}[(c_i^+)^2 - 2c_i^+ + 1] \right\}. \tag{14}$$

Hence the action is

$$S[\alpha(\tau), \pi(\tau)] = \int_0^t d\tau \sum_i \left\{ i\pi_i(\tau)[\partial_\tau \alpha_i(\tau) - v] + v - \frac{\sigma^2}{2} + \sigma^2 i\pi_i(\tau) + \frac{\sigma^2}{2}\pi_i^2(\tau) \right\}. \tag{15}$$

The transformation [4, 5]

$$\pi(\tau) \to \pi(\tau) - il \tag{16}$$

yields an equivalent action:

$$S[\alpha(\tau), \pi(\tau)] = \int_0^t d\tau \sum_i \left\{ i\pi_i(\tau)[\partial_\tau \alpha_i(\tau) - v] + \frac{\sigma^2}{2}\pi_i^2(\tau) \right\} - \sum_i [\alpha_i(0) - \alpha_i(t)]. \tag{17}$$

Inserting equation (17) into equation (10) the probability distribution over coherent states is obtained as:

$$F_\alpha(\alpha, t) = \int_{|\alpha(0)\rangle_N = |F(0)\rangle}^{\alpha(t)=\alpha} \prod_i [d\pi_i(\tau) d\alpha_i(\tau)] \times \exp\left(- \int_0^t d\tau \sum_i \left\{ i\pi_i(\tau)[\partial_\tau \alpha_i(\tau) - v] + \frac{\sigma^2}{2}\pi_i^2(\tau) \right\} \right). \tag{18}$$

Equation (18) is the well known functional integral representation for a stochastic differential equation [9]. That means the $\alpha_i(t)$ obey

$$\partial_t \alpha_i(t) = v + \xi_i(t) \tag{19}$$

where the $\xi_i(t)$ are Gaussian white noise terms with

$$\langle \xi_i(t)\rangle = 0 \qquad \langle \xi_i(t), \xi_j(t')\rangle = \sigma^2 \delta_{ij} \delta(t - t').$$

Provided the characteristic time of the noise ($\tau_n \propto \sigma^{-2}$) is much less than the one for the growth ($\tau_{gr} \propto v^{-1}$), or equivalently $\sigma^2 \gg v$, the standard deviation of α_i is much greater than the one for n_i if the system is in the state $|\alpha\rangle_N$. For large values the n_i can be understood as continuous quantities. Hence, the n_i obey equation (19) as well as the α_i.

$$\partial_t n_i(t) = v + \xi_i(t). \tag{20}$$

Equation (20) is a stochastic differential equation for the occupation numbers. It gives a description equivalent to the rate equation (1). The first and second moments derived from equation (20) are the ones given in equations (12).

The Liouvillian (11) gives a simple model for growing interfaces on a d-dimensional substrate if we identify the interface heights with $\boldsymbol{h} = l\boldsymbol{n}$ (l is the lattice spacing). A more realistic version should take into account diffusion on the surface and the dependence of the growth rate v on $\boldsymbol{h}$ itself. The first extension is introduced by means of the diffusion-Liouvillian L_D [5], the second one by making the simple ansatz $v = \chi\sqrt{1+(\nabla n_i)^2}$. ($\nabla$ is the discrete form of the usual operator here.) That means physically, the deposition rate is proportional to the interface segment spanned between the next neighbours of the site i. We get as Liouvillian:

$$L_i = \sum_i \left\{ \chi[c_i^+ - 1]\sqrt{1+(\nabla n_i)^2} + \frac{\sigma^2}{2}[c_i^+ + (c_i^+)^{-1} - 2] \right\} + L_D \tag{21}$$

with $L_D = \nu c^+ \nabla^2 c$, and ν, χ are constant rates. ν is a measure for the surface tension and χ is proportional to the deposition rate per surface area.

For the action we obtain after the transformation (16):

$$S[\boldsymbol{\alpha}(\tau), \boldsymbol{\pi}(\tau)]$$

$$= \int_0^t d\tau \sum_i \left\{ i\pi_i(\tau)[\partial_\tau \alpha_i(\tau) - \chi\sqrt{1+(\nabla\alpha_i)^2} - \nu\nabla^2\alpha_i] + \frac{\sigma^2}{2}\pi_i^2(\tau) \right\}$$

$$- \sum_i [\alpha_i(0) - \alpha_i(t)]. \tag{22}$$

Following the same arguments as above we get for the heights $h(\boldsymbol{x}, t) = h_i(t)$ ($\boldsymbol{x}$ is the position of the site i):

$$\partial_t h(\boldsymbol{x}, t) = \nu l^2 \nabla^2 h(\boldsymbol{x}, t) + \chi l\sqrt{1+[\nabla h(\boldsymbol{x}, t)]^2} + l\xi(\boldsymbol{x}, t) \tag{23}$$

with

$$\langle \xi(\boldsymbol{x}, t) \rangle = 0 \qquad \langle \xi(\boldsymbol{x}, t), \xi(\boldsymbol{x}', t') \rangle = \sigma^2 l^d \delta(\boldsymbol{x} - \boldsymbol{x}')\delta(t - t').$$

Equation (23) is a stochastic differential equation for the height of an interface growing on a substrate.

Assuming $\nabla h(\boldsymbol{x}, t) \ll 1$ we obtain by expanding the square root in equation (23):

$$\partial_t h(\boldsymbol{x}, t) = \nu l^2 \nabla^2 h(\boldsymbol{x}, t) + \tfrac{1}{2}\chi l[\nabla h(\boldsymbol{x}, t)]^2 + \chi l + l\xi(\boldsymbol{x}, t). \tag{24}$$

Equation (24) is the well known Kardar–Parisi–Zhang equation investigated in many papers (for a review see [8]). However, equation (23) gives a more precise description since the approximation $\nabla h(\boldsymbol{x}, t) \ll 1$ cannot be ensured.

In this paper we have proposed a method for deriving a stochastic differential equation from a rate equation. Contrary to other approaches, e.g. van Kampen's expansion, a Fock space formalism is used which leads immediately to a path integral representation for probabilities. A simple model for particle deposition on a lattice is considered. The derived stochastic differential equation gives exact moments of first and second order. A more realistic model for growing interfaces results in a generalization of the Kardar–Parisi–Zhang equation. The latter one is obtained as an approximation.

Further work on models with coloured noise is in progress.

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