STOCHASTIZATION OF ONE-STEP PROCESSES IN THE OCCUPATIONS NUMBER REPRESENTATION

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ABSTRACT

By the means of the method of stochastization of one-step processes we get the simplified mathematical model of the original stochastic system. We can explore these models by standard methods, as opposed to the original system. The process of stochastization depends on the type of the system under study. We want to get a unified abstract formalism for stochastization of one-step processes. This formalism should be equivalent to the previously introduced. To implement an abstract approach we use the representation of occupation numbers. In this presentation we use the operator formalism. A feature of this formalism is the use of abstract linear operators which are independent from the state vectors. We use the formalism of Green’s functions in order to deal with operators. We get a fully coherent formalism by using the occupation numbers representation. With its help we can get simplified stochastic model of the original system. We demonstrate the equivalence of the occupation number representation and the state vectors representation by using a one-step process example. We have suggested a convenient formalism for unified description of stochastic systems. Also, this method can be extended for the study of nonlinear stochastic systems.

INTRODUCTION

When modeling various physical and technical systems, we often can model them in the form of a one-step processes (see Demidova et al. (2013, 2014); Velieva et al. (2014); Basharin et al. (2009)). Then there is the problem of adequate representation and study of the resulting model. The formalism of stochastization of one-step processes has been developed by our group for quite a long time. But so far, our efforts have been aimed at getting more models than on their investigation. For the statistical systems in addition to representation of the state vectors (combinatorial approach) the representation of the occupation numbers (operator approach) (see Hnatiˇc et al. (2016); Grassberger and Scheunert (1980); T ¨auber (2005); Janssen and T¨auber (2005); Mobilia et al. (2006)) is also used. This representation is especially well suited for the system with a variable number of elements description. In addition, for this representation there are effective methods for solving equations based on the formalism of Green’s functions and perturbation theory.

In this paper, we want to demonstrate the methodology of both approaches.

The structure of the article is as follows. In the first section basic notations and conventions are introduced. The ideology of the method of of stochastization of one-step process and its components are described in the second section. Then the interaction schemes and master equation overview are presented in the next section. The combinatorial method of modelling is discussed in the following section. The operator model approach is presented in the last section, where, in
particular, the algorithm of transition to the occupation number representation is described.

NOTATIONS AND CONVENTIONS

1) The abstract indices notation (see Penrose and Rindler (1987)) is used in this work. Under this notation a tensor as a whole object is denoted just as an index (e.g., \( x^i \)), components are denoted by underlined index (e.g., \( x_i^\alpha \)).

2) We will adhere to the following agreements. Latin indices from the middle of the alphabet (\( i, j, k \)) will be applied to the space of the system state vectors. Latin indices from the beginning of the alphabet (\( \alpha \)) will be related to the Wiener process space. Greek indices (\( \alpha \)) will set a number of different interactions in kinetic equations.

GENERAL REVIEW OF THE METHODOLOGY

Our methodology is completely formalized in such a way that it is sufficient when the original problem is formulated accordingly. It should be noted that the most of the models under our study can be formalized as a one-step process (see van Kampen (2011); Gardiner (1985)). In fact, for this type of models we developed this methodology, but it may be expanded for other processes.

First we transform our model to the one-step process (see Fig. 1). Next, we need to formalize this process in the form of interaction schemes (see Demidova et al. (2013, 2014); Hnatič et al. (2016)).

Each scheme has its own interaction semantics. Semantics leads directly to the master equation (see van Kampen (2011); Gardiner (1985)). However, the master equation has usually rather complex structure that makes it difficult for direct study and solution. Our technique involves two possibilities (see Fig. 2):

- computational approach — the solution of the master equation with help of perturbation theory;
- modeling approach — the approximate models are obtained in the form of Fokker–Planck and Langevin equations.

The computational approach allows to obtain a concrete solution for the studied model. In our methodology, this approach is associated with perturbation theory (see Hnatič et al. (2013); Hnatich and Honkonen (2000); Hnatich et al. (2011)). Methodologically, this method is quite simple. Each expansion element appears in the form of of Feynman diagrams. However, with increasing order of the expansion, the number of Feynman diagrams increases rapidly and can reach tens or hundreds of thousands. It is quite natural that this should involve high-performance computing.

The model approach provides a model that is convenient to study numerically and qualitatively. In addition, this approach assumes the iterative process of research: the obtained approximate model can be specified and changed, which leads to the correction of initial interaction schemes.

In this article we will describe the model approach.

There are two ways of building the master equation:

- combinatorial approach (see Fig. 3);
- operator approach (see Fig. 4).

In the combinatorial approach, all operations are performed in the space of states of the system, so we deal with a particular system throughout manipulations with the model.

For the operator approach we can abstract from the specific implementation of the system under study. We are working with abstract operators. We return to the state space only at the end of the calculations. In addition, we choose a particular operator algebra on the basis of symmetry of the problem.

These two approaches are belong to different paradigms of physical theories construction. Accordingly, they are complementary. Some constructions are simpler in one approach, others are simpler in another. For example, in the combinatorial approach, the process of obtaining the approximate models is more convenient, but not more easy. For perturbation theory it is easier to expand in a series the master equation by using the operator formalism. In addition, the operator formalism is suitable for describing the transient processes and non-stationary statistical systems.

Interaction schemes

The system state is defined by the vector \( \varphi^i \in \mathbb{R}^n \), where \( n \) is system dimension. The operator \( I_j^i \in \mathbb{R}^n_0 \times \mathbb{R}^n_0 \) describes the state of the system before the interaction, the operator \( F_j^i \) \( \in \mathbb{R}^n_0 \times \mathbb{R}^n_0 \) describes the state of the system after the interaction. The result of interaction is the system transition from one state to another one.

There are \( s \) types of interaction in our system, so instead of \( I_j^i \) and \( F_j^i \) operators we will use operators \( I_j^{i\alpha} \) \( \in \mathbb{R}^n_0 \times \mathbb{R}^n_0 \times \mathbb{R}^n_0 \) and \( F_j^{i\alpha} \) \( \in \mathbb{R}^n_0 \times \mathbb{R}^n_0 \times \mathbb{R}^n_0 \).

The interaction of the elements will be described by interaction schemes, which are similar to schemes of chemical kinetics Waage and Gulberg (1986); Gorban and Yablonsky (2015):

\[
I_j^{i\alpha} \varphi^i \xrightarrow{+k_{\alpha}} F_j^{i\alpha} \varphi^i, \quad \alpha = 1, s, \tag{1}
\]

the Greek indices specify the number of interactions and Latin are the system order. The coefficients \( k_{\alpha} \) and \( k_{\alpha} \) have meaning intensity (speed) of interaction.

The state transition is given by the operator:

\[
l_j^{i\alpha} = F_j^{i\alpha} - I_j^{i\alpha}. \tag{2}
\]

\( ^2 \)In quantum field theory the path integrals approach can be considered as an analogue of the combinatorial approach and the method of second quantization as analog of the operator approach.

\( ^3 \)For brevity, we denote the module over the field \( \mathbb{R} \) just as \( \mathfrak{L} \). Accordingly, \( \mathfrak{L}, \mathfrak{N}, \mathfrak{N}_0, \mathfrak{N}_+ \) are modules over rings \( \mathbb{N}, \mathbb{N}_0 \) (cardinal numbers with 0), \( \mathbb{N}_+ \) (cardinal numbers without 0).

\( ^4 \)The component dimension indices take on values \( i, j = 1, n \)

\( ^5 \)The component indices of number of interactions take on values \( \alpha = 1, s \)
Thus, one step interaction $\alpha$ in forward and reverse directions can be written as
\[
\varphi^i \rightarrow \varphi^j + r_{ij}^\alpha \varphi^i,
\]
\[
\varphi^i \rightarrow \varphi^j - r_{ij}^{-\alpha} \varphi^i.
\]

We can also write (1) not in the form of vector equations but in the form of sums:
\[
I_{ij}^\alpha \varphi^i \delta_i = \frac{+k_{ij}^\alpha}{-k_{ij}^\alpha} F_{ij}^\alpha \varphi^j \delta_i,
\]
where $\delta_i = (1, \ldots, 1)$.

Also the following notation will be used:
\[
I_{ij}^\alpha := I_{ij}^\alpha \delta_i, \quad F_{ij}^\alpha := F_{ij}^\alpha \delta_j, \quad r_{ij}^\alpha := r_{ij}^{-\alpha} \delta_j.
\]

**The master equation**

For the system description we will use the master equation,\(^6\) which describes the transition probabilities for Markov process (see van Kampen (2011); Gardiner (1985)):

\[
\frac{\partial p_n(t)}{\partial t} = \sum_{m} \left[ w_{nm} p_m(t) - w_{mn} p_n(t) \right],
\]
where $p_n(t)$ is the probability of transition from the state $n$ at time $t$, $w_{nm}$ is the probability of transition from the state $m$ into the state $n$ per unit time.

There are two types of system transition from one state to another (based on one–step processes) as a result of system elements interaction: in the forward direction $(\varphi^i + r_{ij}^\alpha \varphi^j)$ with the probability $^+s_{ij}^\alpha(\varphi^j)$ and in the opposite direction $(\varphi^i - r_{ij}^{-\alpha} \varphi^j)$ with the probability $^-s_{ij}^\alpha(\varphi^j)$ (fig. 1). The matrix of transition probabilities has the form:

\[
w_{ij}^\alpha(\varphi^i, \psi, t) = ^+s_{ij}^\alpha(\varphi^i) \delta_{\alpha, \psi} + ^-s_{ij}^\alpha(\varphi^i) \delta_{\alpha, \psi} - 1, \quad \alpha = 1, \ldots, n,
\]
where $\delta_{i,j}$ is Kronecker delta.

Thus, the general form of the master equation for the state vector $\varphi^i$, changing by steps with length $r_{ij}^\alpha \varphi^j$, is:

\[
\frac{\partial p(\varphi, t)}{\partial t} = \sum_{\alpha=1}^{n} \left\{ ^+s_{ij}^\alpha(\varphi^i + r_{ij}^\alpha, t) p(\varphi^i + r_{ij}^\alpha, t) + ^-s_{ij}^\alpha(\varphi^i - r_{ij}^{-\alpha}, t) p(\varphi^i - r_{ij}^{-\alpha}, t) - \left[ ^+s_{ij}^\alpha(\varphi^i) + ^-s_{ij}^\alpha(\varphi^i) \right] p(\varphi^i, t) \right\}. \tag{5}
\]

**COMBINATORIAL APPROACH**

We will obtain the function $^+s_{ij}^\alpha$ and $^-s_{ij}^\alpha$ for equation (5) with use of combinatorial approach.

**The transition probabilities**

The transition rates $^\alpha s_{ij}$ and $^-s_{ij}^\alpha$ are proportional to the number of ways of choosing the number of arrangements of
\( \varphi \) to \( I^{\alpha} \) (denoted as \( A_{\varphi}^{\alpha} \)) and to \( F^{\alpha} \) (denoted as \( A_{\varphi}^{\alpha} \)) and defined by:

\[
\begin{align*}
+ s_{\alpha} & = + k_{\alpha} \prod_{i=1}^{n} A_{\varphi}^{\alpha} = + k_{\alpha} \prod_{i=1}^{n} \left( \varphi_{i}^{\alpha} - I^{\alpha}_{i} \right)!, \\
- s_{\alpha} & = - k_{\alpha} \prod_{i=1}^{n} A_{\varphi}^{\alpha} = - k_{\alpha} \prod_{i=1}^{n} \left( \varphi_{i}^{\alpha} - F^{\alpha}_{i} \right)!
\end{align*}
\]  

(6)

Replacing in (6) the \( \varphi(\varphi - 1) \cdots (\varphi - (n - 1)) \)-type combinations on \( (\varphi)^{n} \) we obtain for Fokker–Planck equation\(^{7}\):

\[
\begin{align*}
+ \varphi s_{\alpha} & = + k_{\alpha} \prod_{i=1}^{n} (\varphi_{i})^{I^{\alpha}_{i}} , \\
- \varphi s_{\alpha} & = - k_{\alpha} \prod_{i=1}^{n} (\varphi_{i})^{F^{\alpha}_{i}} .
\end{align*}
\]

Fokker–Planck equation

The Fokker–Planck equation is a special case of the master equation and can be regarded as its approximation. We can get through the expansion of the master equation in a series up to the second order. We will use the decomposition of the Kramers–Moyal (see Gardiner (1985)) (for simplicity it is written for the one-dimensional case):

\[
\frac{\partial p(\varphi, t)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^{n}}{n!} \frac{\partial^{n}}{\partial \varphi^{n}} \left[ \xi^{n}(\varphi)p(\varphi, t) \right],
\]

where

\[
\xi^{n}(\varphi) = \int (\psi - \varphi)^{n} w(\psi|\varphi) \, d\psi .
\]

By dropping the terms with order higher than the second one, we obtain the Fokker–Planck equation:

\[
\frac{\partial p(\varphi, t)}{\partial t} = - \frac{\partial}{\partial \varphi} \left[ A(\varphi)p(\varphi, t) \right] + \frac{\partial^{2}}{\partial \varphi^{2}} \left[ B(\varphi)p(\varphi, t) \right],
\]

and for multivariate case

\[
\begin{align*}
\frac{\partial p(\varphi^{k}, t)}{\partial t} & = - \frac{\partial}{\partial \varphi^{k}} \left[ A^{k}(\varphi^{k})p(\varphi^{k}, t) \right] + \\
& + \frac{1}{2} \frac{\partial^{2}}{\partial \varphi^{k} \partial \varphi^{j}} \left[ B^{ij}(\varphi^{k})p(\varphi^{k}, t) \right],
\end{align*}
\]

(7)

where

\[
\begin{align*}
A^{i} & := A^{i}(\varphi^{k}) = r^{i}_{\alpha} \left[ + \varphi s_{\alpha} - \varphi s_{\alpha} \right] , \\
B^{ij} & := B^{ij}(\varphi^{k}) = r^{i}_{\alpha} r^{j}_{\beta} \left[ + \varphi s_{\alpha} - \varphi s_{\alpha} \right].
\end{align*}
\]

(8)

As can be seen from the (8), the coefficients of the Fokker–Planck equation can be obtained directly from the (2) and (6), that is, in this case, it is not necessary to write down the master equation.

\(^{7}\)This change corresponds to a series expansion.

Langevin equation

The Langevin equation which corresponds to the Fokker–Planck equation:

\[
d\varphi^{i} = a^{i} \, dt + b^{i}_{\alpha} \, dW^{\alpha},
\]

(9)

where \( a^{i} := a^{i}(\varphi^{k}) , \ b^{i}_{\alpha} := b^{i}_{\alpha}(\varphi^{k}) , \ \varphi^{i} \in \mathbb{R}^{n} \) is the system state vector, \( W^{\alpha} \in \mathbb{R}^{m} \) is the m-dimensional Wiener process\(^{8}\). Latin indices from the middle of the alphabet will be applied to the system state vectors (the dimensionality of space is \( n \)), and Latin indices from the beginning of the alphabet denote the variables related to the Wiener process vector (he dimensionality of space is \( m \leq n \)).

The connection between the equations (7) and (9) is expressed by the following relationships:

\[
A^{i} = a^{i} , \quad B^{ij} = b^{i}_{\alpha} b^{j}_{\alpha} .
\]

It can be seen that the second term of the Langevin equation is a square root, which has a complicated form in the multidimensional case. However, we note that is often used is the square of the second term of the Langevin equation, so often calculate the root is not required.

OPERATOR APPROACH

Occupation numbers representation

Occupation number representation is the main language in the description of many-body physics. The main elements of the language are the wave functions of the system with information about how many particles are in each single-particle state. The creation and annihilation operators are used for system states change. The advantages of this formalism are following:

• it is possible to consider systems with a variable number of particles (non-stationary systems);
• system statistics (Fermi–Dirac or Bose–Einstein) is automatically included in the commutation rules for the creation and annihilation operators;
• this is the second major formalism (along with the path integral) for the quantum perturbation theory description.

The method of application of the formalism of second quantization for the non-quantum systems (statistical, deterministic systems) was studied in a series of articles (see Doi (1976a,b); Grassberger and Scheunert (1980); Peliti (1985)).

The Dirac notation is commonly used for occupation numbers representation recording.

Dirac notation

This notation is proposed by P. A. M. Dirac\(^{9}\) (see Dirac (1939)). Under this notation, state of the system is described by an element of the projective Hilbert space \( \mathcal{H} \). The vector

\(^{8}\)The Wiener process is realized as \( dW = \epsilon \sqrt{dt} \), where \( \epsilon \sim \mathcal{N}(0,1) \) — the normal distribution with mean 0 and variation 1.

\(^{9}\)The notation is based on the notation, proposed by G. Grassmann in 1862 (see Cajori, 1929, p. 134)).
\( \varphi^i \in \mathcal{H} \) is defined as \( |i\rangle \), and covariant vector (covector) \( \varphi_i \in \mathcal{H}^* := \mathcal{H}_0 \) is defined as \( \langle i| \). Conjunction operation is used for raising and lowering of indices:\(^{10}\)

\[
\varphi_i^\dagger := \varphi_i = (\varphi^i)^\dagger \equiv \langle i| = |i\rangle^\dagger. \tag{10}
\]

The scalar product is as follows:

\[
\varphi_i \varphi_i^\dagger \equiv \langle i|i \rangle.
\]

The tensor product is:

\[
\varphi_j \varphi_i^\dagger \equiv |i\rangle \langle j|.
\]

However, this notation (10) is normally used for some dedicated vectors, such as basis \((\delta^i_j)\) or eigenvectors. Then conventional vectors using the notation of the following form:

\[
|\varphi\rangle \equiv \varphi^i, \quad \langle i|\varphi \rangle \equiv \varphi_i \delta_i^j = \varphi^j.
\]

Linear operators are usually used for operations with vectors. Let \( A_j^i : \mathcal{H} \to \mathcal{H}_0 \) be a linear operator. Then the inner product will be as follows:

\[
A_j^i \varphi_i \psi^j \equiv \langle \varphi|A|\psi \rangle.
\]

Component representation of a linear operator can be written as follows:

\[
A^i_j = A_j^i \delta^i_\lambda \delta^j_\lambda \equiv \langle i|A|j \rangle.
\]

**Creation and annihilation operators**

The transition to the space of occupation numbers is not a unitary transformation. However, the algorithm of transition (specific to each task) can be constructed.

Let’s write the master equation (4) in the occupation number representation. We will consider a system that does not depend on the spatial variables. For simplicity, we consider the one-dimensional version.

Let’s denote in (4) the probability that there are \( n \) particles in our system as \( \varphi_n \):

\[
\varphi_n := p_n(\varphi, t).
\]

The vector space \( \mathcal{H} \) consists of states of \( \varphi \).

We introduce a scalar product, exclusive (\( \langle | \rangle_{ex} \)) and inclusive (\( \langle | \rangle_{in} \)). Let \( |n\rangle \) are basis vectors.

\[
\langle \varphi|\psi \rangle_{ex} = \sum_n n! p_n(\varphi)p^n(\psi); \tag{11}
\]

\[
\langle \varphi|\psi \rangle_{in} = \sum_n \frac{1}{k!} n_k^i(\varphi)n_k^i(\psi). \tag{12}
\]

There \( n_k \) are factorial moments:

\[
n_k(\varphi) = \langle n(n - 1) \cdots (n - k + 1) \rangle = \frac{\partial^k}{\partial z^k} G(z, \varphi)|_{z=1}, \tag{13}
\]

\( G \) is generating function:

\[
G(z, \varphi) = \sum_n z^n p_n(\varphi). \tag{14}
\]

Normalizing for the generating function is obvious. Let \( z = 1 \) in equation (14). Then

\[
\sum_n p_n(\varphi) = 1, \quad G(1, \varphi) = 1, \quad n_0(\varphi) = 1.
\]

From \( p_n(m) = \delta^m_m \) and (11) we can obtain:

\[
\langle n|m \rangle_{ex} = n! \delta^m_m. \tag{15}
\]

The state vectors:

\[
|\varphi\rangle = \sum_n p_n(\varphi) |n\rangle = \sum_n \varphi_n |n\rangle := \varphi_n |n\rangle. \tag{16}
\]

In view of (15) the following expression may be written:

\[
\varphi_n = \frac{1}{n!} \langle n|\varphi \rangle_{ex}.
\]

Let’s use creation and annihilation operators:

\[
\pi |n\rangle = |n + 1\rangle, \quad a |n\rangle = |n - 1\rangle
\]

and commutation rule:\(^{11}\)

\[
[a, \pi] = 1. \tag{18}
\]

If the form of scalar product is (11) then with the help of (18) it is obviously that the our system is described by Bose–Einstein statistics.

From the relation (15) we obtain:

\[
\langle m|a^\dagger |n\rangle_{ex} = \langle m|\pi |n\rangle_{ex},
\]

and for the scalar product (11) the following statement is valid:

\[
a^\dagger = \pi.
\]

Now we can write the inclusive scalar product from (14) and (13):

\[
p_n(\varphi) = \frac{1}{n!} \langle n|\varphi \rangle_{ex} = \frac{1}{n!} (0|a^n|\varphi \rangle_{ex},
\]

\[
n_k(\varphi) = \langle 0|\exp(a) a^k |\varphi \rangle_{ex}.
\]

Taking into account the (12), we obtain the inclusive scalar product

\[
\langle \varphi|\psi \rangle_{in} = \langle \varphi|\exp(\pi) \exp(a)|\psi \rangle_{ex}.
\]

Then the expressions (19) will take the following form:

\[
p_n(\varphi) = \frac{1}{n!} (0|\exp(-a) a^n |\varphi \rangle_{in},
\]

\[
n_k(\varphi) = (0|a^k |\varphi \rangle_{in} = (k|\varphi \rangle_{in}.
\]

\(^{10}\)In this case, we use Hermitian conjugation \( \bullet^\dagger \). The sign of the complex conjugate \( \bullet^* \) in this entry is superfluous.

\(^{11}\)In fact, \( a\pi |n\rangle - \pi a |n\rangle = (n + 1) |n\rangle - n |n\rangle = |n\rangle. \)
The Liouville operator

In the occupation numbers formalism the master equation becomes the Liouville equation:

\[ \frac{\partial}{\partial t} \varphi(t) = L |\varphi(t)\rangle. \]  

(20)

The Liouville operator \( L \) satisfies the relation:

\[ \langle 0 | L = 0. \]

From (4), (16), (17) and (20) we obtain:

\[ \frac{\partial p_n}{\partial t} = \frac{1}{n!} \left\langle n \left| \frac{\partial}{\partial t} \right| \varphi \right\rangle = \frac{1}{n!} \langle n | L |\varphi\rangle \equiv \]

\[ \sum_{m} [w_{nm}p_m - w_{mn}p_n], \]

The Liouville equation (20) in the form of a single equation writes down the master equations (4) for different values of \( n \).

The following Liouville operator corresponds to the scheme (1):

\[ L = \sum_{\alpha} \left[ + k_+ \left( (\pi_2)^{F_{\alpha}} - (\pi_2)^{I_{\alpha}} \right) (a_2)^{F_{\alpha}} + 
\right. \]

\[ \left. + - k_- \left( (\pi_2)^{I_{\alpha}} - (\pi_2)^{F_{\alpha}} \right) (a_2)^{I_{\alpha}} \right]. \]  

(21)

As we can see, in the case of the occupation numbers
formalism (21) the schemes of interaction encode the system under study in more universal and transparent way than in the representation of the state vectors (6).

CONCLUSIONS

We presented a preliminary overview of the use of the occupation numbers representation for the record of models describing stochastic statistical systems. However, the model approach does not always present the advantages of described method. We assume that the advantages of the method will reveal most explicitly when computation approach is used.

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