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Quantum Field Theory Approach to the Analysis of One-Step Models

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During development of methods for stochastization of one-step processes the attention was focused on obtaining the stochastic equations in the form of the Langevin, since this form of stochastic equations is most usual in the construction and study of one-step processes models. When applying the method there is the problem of justifying the transition from master equation to the Fokker–Planck equation for the different versions of the model. However, the forms of partial differential equations (master equation and the Fokker–Planck equation) wider description of the model to researchers. It is proposed to treat these equations with the help of perturbation theory in the framework of quantum field theory. For this purpose the methodology was described and the analytical software complex was constructed to write down put the main kinetic equation in the operator form in the Fock representation. To solve the resulting equation the software complex generates Feynman diagrams for the corresponding order of perturbation theory. The FORM system was applied as a system of symbolic computation. Selecting FORM as the CAS is reasonable because that the given computer algebra system allows for symbolic computation, using the resources of high-performance computing. In particular, it is possible to use parallel computing technologies such as OpenMP and MPI.

Key words and phrases: algebraic biology, stochastic differential equations; master equation; Fokker–Planck equation; population models; computer algebra software; FORM system.

1. Introduction

The process of stochastization of one-step processes results in three kinds of differential equations: the master equation, the equation of the Fokker–Planck type and the stochastic differential equation (the Langevin equation). The last two equations are obtained as an approximate version of the master equation. And if the stochastic differential equations solving methods are well known (e.g., stochastic Runge–Kutta method), then the solution of partial differential equations is a certain problem.

It is proposed to use perturbation methods, namely the methods developed in quantum field theory, for these equations solution.

The main aim of this work is to develop the software complex to obtain the analytical form for all three types of differential equations describing the model. The Feynman diagrams are calculated for the master equation for the corresponding perturbation theory order.

A well-known model of logistic population growth (model Verhulst) is used for the presented system. The structure of the article is as follows. In the section 2 basic notation and conventions are introduced. The section 3 contains a summary of the perturbation theory. The Section 4 contains a brief introduction to the method

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of stochastization of one-step processes and the technology of reducing the above equations to the form of the Liouville equation. Further, in the section 5 the model under study is described. The section 6 describes the ideology of software package development.

2. Notations and Conventions

1. The abstract indices notation [1] 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., $x^{\underline{i}}$).
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 (a) will be related to the Wiener process space. Greek indices (α) will set a number of different interactions in kinetic equations.
3. A Dot over a symbol denotes derivative with time.

3. Elements of Perturbation Theory

In perturbation theory, the Hamiltonian is written as the sum of $H = H_0 + H_{\text{int}}$, where H_0 is an unperturbed part and H_{int} is a perturbed one [2]. We will use the Heisenberg's representation of unperturbed problem. Time-dependent eigenstates of the unperturbed Hamiltonian H_0 are used as the basis:

$$|\alpha\rangle\,(t) = e^{E_\alpha t}\,|\alpha\rangle\,, \tag{1}$$

where E_α is a spectrum of H_0. The form of Schrödinger equation written in this basis:

$$\frac{\partial\psi}{\partial t} = H_{\text{int}}(t)\psi, \tag{2}$$

where $H_{\text{int}}(t) = e^{H_0 t} H_{\text{int}} e^{H_0 t}$, and ψ are given in the interaction representation. A formal decision is written through the S–matrix, $\psi(t) = S(t)\psi(0)$, which is presented by the chronological exponential:

$$S(t) = T\exp\left[\int_0^t H_{\text{int}}(t')\mathrm{d}t'\right] = \sum_{n=0}^{\infty}\int_0^t\int_0^{t_1}\dots\int_0^{t_{n-1}} H_{\text{int}}(t_1)\dots H_{\text{int}}(t_n)\mathrm{d}t_n\dots\mathrm{d}t_1, \tag{3}$$

where $0 < t_n < \ldots < t_1 < t_0$. In multiparticle case we should use the ψ–operators, then the terms of (3) becomes polynomials in the operators of creation and destruction.

Let's introduce the chronological product of operators, also known as T–ordered product. During operators T–ordering they are rearranged so that the time moments, in which the operator is taken, increased from right to left. Let's write the expression (3) with T–ordering.

$$S(t) = \sum_{n=0}^{\infty}\frac{1}{n!}T\left(\int_0^t H_{\text{int}}(t')\mathrm{d}t'\right)^n. \tag{4}$$

The main object of the diagram technique is the Green's function. It is defined by ψ–operators, given in the interaction's view:

$$\psi_\alpha(x) = e^{H_0 t}\psi_\alpha(r)e^{H_0 t}, \quad \psi^+_\alpha(x) = e^{H_0 t}\psi^+_\alpha(r)e^{H_0 t}, \tag{5}$$

where x is a set of variables —coordinates r and time t; α is a spin index.

The causal Green's function is the average of the chronological product of ψ–operators:

$$G^c_{\alpha\beta}(x,x') = \langle T\psi_\alpha(x)\psi^+_\beta(x')\rangle, \tag{6}$$

where the brackets $\langle\ldots\rangle$ denote the matrix element $\langle S_0\rangle^{-1}\langle 0|\ldots|0\rangle$, which was taken over the ground state of the system with the Hamiltonian H_0.

4. One-Step Processes

One-step processes and birth–death processes [3–5] are defined as Markov processes with continuous time and integer state. The transitions are possible only between adjacent states (see fig. 1).

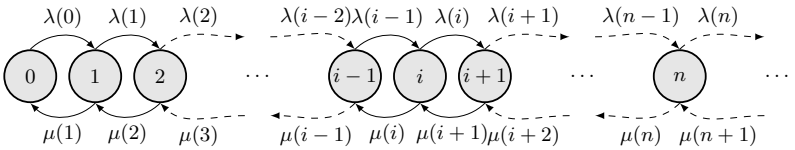

Figure 1. One-step process

The coefficient $\lambda(n)$ is the probability that during unit time a transition from the state of n into $n+1$ will occurs and the coefficient $\mu(n)$ is the probability of transition into the state of $n-1$ during unit time.

The state of the system will be described by a state vector $\left|n^i\right\rangle \in \mathbb{R}^n$, where n is the dimension of the system (under the state vector we mean the set of mathematical values, which fully describe the system). The operator $I^i_j \in \mathbb{Z}^n_{\geqslant 0} \times \mathbb{Z}^n_{\geqslant 0}$ defines the state of the system before the interaction, the operator $F^i_j \in \mathbb{Z}^n_{\geqslant 0} \times \mathbb{Z}^n_{\geqslant 0}$ defines the state of the system after the interaction. As a result of interaction the transition to another state of the system occurs.

There are s kinds of different interactions in the system, $s \in \mathbb{Z}_+$. So, instead of operators I^i_j and F^i_j the operators $I^{i\alpha}_j \in \mathbb{Z}^n_{\geqslant 0} \times \mathbb{Z}^n_{\geqslant 0} \times \mathbb{Z}^s_+$ and $F^{i\alpha}_j \in \mathbb{Z}^n_{\geqslant 0} \times \mathbb{Z}^n_{\geqslant 0} \times \mathbb{Z}^s_+$ will be used.

The interaction of the system's elements will be described by the schemes of interaction, similar to schemes of chemical kinetics [6, 7]:

$$I^{i\alpha}_j \left|n^j\right\rangle \underset{k^-_\alpha}{\overset{k^+_\alpha}{\rightleftharpoons}} F^{i\alpha}_j \left|n^j\right\rangle, \tag{7}$$

here the Greek indices specify the number of interactions and Latin indices specify the dimension of the system.

The state change is set by the operator

$$R^{i\alpha}_j = F^{i\alpha}_j - I^{i\alpha}_j. \tag{8}$$

Consequently, the one-step interaction α in direct and reverse directions can be written as:

$$\left|n^i\right\rangle \to \left|n^i\right\rangle + R^{i\alpha}_j \left|n^j\right\rangle, \quad \left|n^i\right\rangle \to \left|n^i\right\rangle - R^{i\alpha}_j \left|n^j\right\rangle. \tag{9}$$

The expression (7) may be represented not in the form of vector equations but as sums:

$$I^{i\alpha}_j \left|n^j\right\rangle \delta_i \underset{k^-_\alpha}{\overset{k^+_\alpha}{\rightleftharpoons}} F^{i\alpha}_j \left|n^j\right\rangle \delta_i, \tag{10}$$

where $\delta_i = (1, \ldots, 1)$.

We shall use the following notation:

$$I^{i\alpha} := I^{i\alpha}_j \delta^j, \quad F^{i\alpha} := F^{i\alpha}_j \delta^j, \quad R^{i\alpha} := R^{i\alpha}_j \delta^j. \tag{11}$$

The transition probabilities per unit time from the state of $|n^a\rangle$ into the state $|n^i\rangle + R^{i\alpha}_{\underline{j}} |n^j\rangle$ (into the state $|n^i\rangle - R^{i\alpha}_{\underline{j}} |n^j\rangle$) are proportional to the number of ways to select a combination of $I^{i\alpha}$ taken $|n^i\rangle$ (combination of $F^{i\alpha}$ taken $|n^i\rangle$) and are given by:

$$\begin{aligned} \lambda_{\underline{\alpha}}(k^+_\alpha, |n^i\rangle) &= k^+_{\underline{\alpha}} \prod_{\underline{i}=1}^{n} \frac{n^{\underline{i}}!}{(n^{\underline{i}} - I^{i\alpha})!}, \\ \mu_{\underline{\alpha}}(k^-_\alpha, n^i) &= k^-_{\underline{\alpha}} \prod_{\underline{i}=1}^{n} \frac{n^{\underline{i}}!}{(n^i - F^{i\alpha})!}. \end{aligned} \tag{12}$$

Thus, the general form of the master equation for the state vector $|n^i\rangle$, changing by steps of length $R^{i\alpha}_j n^j$, has the form:

$$\begin{aligned} \frac{\partial p(n^i, t)}{\partial t} = \sum_{\underline{\alpha}} \Big\{ \Big[\mu_{\underline{\alpha}}(k^-_\alpha, n^i)(n^i + R^{i\alpha}_{\underline{\cdot}}, t) p(n^i + R^{i\alpha}_{\underline{\cdot}}, t) - \lambda_{\underline{\alpha}}(k^+_\alpha, n^i)(n^i) p(n^i, t) \Big] + \\ + \Big[\lambda_{\underline{\alpha}}(k^+_\alpha, n^i)(n^i - R^{i\alpha}_{\underline{\cdot}}, t) p(n^i - R^{i\alpha}_{\underline{\cdot}}, t) - \mu_{\underline{\alpha}}(k^-_\alpha, n^i)(n^i) p(n^i, t) \Big] \Big\}. \end{aligned} \tag{13}$$

In order of notation reduction the operators of creation $\varepsilon^\dagger$ and operators of death ε are introduced. They are defined the following way:

$$\varepsilon^\dagger f(n) = f(n+1), \quad \varepsilon f(n) = f(n-1). \tag{14}$$

The commutation relations are defined as follows:

$$\left[\varepsilon(n), \varepsilon^\dagger(n')\right] = \delta(n - n'), \quad [\varepsilon(n), \varepsilon(n')] = 0, \quad \left[\varepsilon^\dagger(n), \varepsilon^\dagger(n')\right] = 0. \tag{15}$$

With the help of the creation and death operators the basic kinetic equation for the one-step processes can be written as:

$$\frac{\partial p\left(n^i, t\right)}{\partial t} = \sum_{\underline{\alpha}} \left\{ (\varepsilon^\dagger_{\underline{\alpha}} - 1) \mu_{\underline{\alpha}}\left(k^-_\alpha, n^i\right) p\left(n^i, t\right) + (\varepsilon_{\underline{\alpha}} - 1) \lambda_{\underline{\alpha}}\left(k^+_\alpha, n^i\right) p(n^i, t) \right\}. \tag{16}$$

In order to apply the operator method of perturbation theory we will use the operators of creation–death in Fock representation ($a^\dagger$ and a operators) [8]. Their presentations are well known. For simplicity, for the one-dimensional case the ratio of these operators has the form:

$$\begin{aligned} a^\dagger |n\rangle &= |n+1\rangle, \\ a |n\rangle &= n |n-1\rangle, \\ a^\dagger a |n\rangle &= n |n\rangle, \\ \left[a^\dagger, a\right] &= 1, \\ \langle n | m \rangle &= \delta_{nm}. \end{aligned} \tag{17}$$

Let's introduce a state vector $|\nu\rangle$ as follows:

$$|\nu\rangle = \sum_{n=0}^{\infty} p(n,t)\,|n\rangle\,. \tag{18}$$

Let's assume that the operators of creation–death act only on the vector $|n\rangle$, but not at $p(n,t)$:

$$\begin{aligned} a^{\dagger}p(n,t)\,|n\rangle &= p(n,t)\,|n+1\rangle\,,\\ ap(n,t)\,|n\rangle &= np(n,t)\,|n-1\rangle\,,\\ a^{\dagger}ap(n,t)\,|n\rangle &= np(n,t)\,|n\rangle\,. \end{aligned} \tag{19}$$

The following operator equation is obtained by multiplying the master equation by $|n\rangle$ and by summing over n:

$$\frac{\mathrm{d}\,|\nu\rangle}{\mathrm{d}t} = L(a^{\dagger},a)\,|\nu\rangle\,. \tag{20}$$

The Liouville operator $L(a^{\dagger},a)$ will be used in calculations under perturbation theory.

5. Verhulst Model

In order to demonstrate the method, let's consider the Verhulst model [9–11] which describes limited growth [1]:

$$\frac{\partial n}{\partial t} = \lambda n - \beta n - \gamma n^2. \tag{21}$$

Next, we will construct a stochastic model for the system with the help of the method described in the second chapter. At first the schemes of interaction are presented:

$$\begin{aligned} N &\underset{\gamma}{\overset{\lambda}{\rightleftharpoons}} 2N,\\ N &\xrightarrow{\beta} 0. \end{aligned} \tag{22}$$

The first ratio means the immediate reproduction of an individual who eats unit of food, but it also means the competition between individuals. The second ratio means death of an individual.

According to (12) the intensity of the transition is defined:

$$\begin{aligned} \lambda_1(n) &= \lambda\frac{n!}{(n-1)!} = \lambda n,\\ \mu_1(n) &= \gamma\frac{n!}{(n-2)!} = \gamma n(n-1) \sim \gamma n^2,\\ \lambda_2(n) &= \beta\frac{n!}{(n-1)!} = \beta n. \end{aligned} \tag{23}$$

Then the master equation takes the following form:

$$\begin{aligned} \frac{\partial p(n,t)}{\partial t} = &-(\lambda n + \beta n + \gamma n^2)p(n,t) +\\ &+ (\beta(n+1) + \gamma(n+1)^2)p(n+1,t) + \lambda(n-1)p(n-1,t). \end{aligned} \tag{24}$$

[1] The attractiveness of this model is that it is one-dimensional and nonlinear.

By multiplying (24) by $|n\rangle$ and summing over n the next formula is obtained [12–17]:

$$\frac{\partial |\nu\rangle}{\partial t} = \sum_n \frac{\partial}{\partial t}[|n\rangle\, p(n,t)] = \sum_n \left[\left(\beta(n+1) + \gamma(n+1)^2\right) p(n+1,t)\,|n\rangle\right] + \\ + \sum_n \left[\lambda(n-1)p(n-1,t)\,|n\rangle\right] - \sum_n \left[\left(\beta n + \lambda n + \gamma n^2\right) p(n,t)\,|n\rangle\right]. \quad (25)$$

The following substitutions are introduced in order to obtain the Fock representation (17):

$$\begin{aligned} np(n,t)\,|n\rangle &\to a^\dagger a p(n,t)\,|n\rangle\,, \\ p(n,t)\,|n+1\rangle &\to a^\dagger p(n,t)\,|n\rangle\,, \\ np(n,t)\,|n-1\rangle &\to a p(n,t)\,|n\rangle\,. \end{aligned} \quad (26)$$

By substituting (26) in (25) and leaving only the terms in $|n\rangle$ the following formula is obtained:

$$\sum_n \frac{\partial}{\partial t}[|n\rangle\, p(n,t)] = \\ = \left[\beta a - \beta a^\dagger a + \gamma a a^\dagger a - \gamma a^\dagger a a^\dagger a + \lambda a^\dagger a^\dagger a - \lambda a^\dagger a\right] \sum_n p(n,t)\,|n\rangle\,. \quad (27)$$

Similarly to (20) the Liouville operator is written:

$$L(a^\dagger, a) = \beta a - \beta a^\dagger a + \gamma a a^\dagger a - \gamma a^\dagger a a^\dagger a + \lambda a^\dagger a^\dagger a - \lambda a^\dagger a = \\ = \lambda\left(a^\dagger - 1\right) a^\dagger a + \beta\left(1 - a^\dagger\right) a + \gamma\left(1 - a^\dagger\right) a a^\dagger a. \quad (28)$$

6. Implementation of the Method

The FORM program [18–20] was selected as an environment for software system implementation. Unlike others, this computer algebra system is focused not on interactive work with user but on a batch processing. Due to this, it became possible to remove such inherent disadvantages of conventional computer algebra systems as restrictions on the volumes of computations, slowness. The FORM system supports different technologies of parallel and distributed computing [21], such as multi-thread approach, as well as MPI (multiple implementations) technology. The result of these properties of the package is that it is often used as a back-end for the other (mostly interactive) computer algebra systems [22].

We drew attention to this package also because it is being used for the calculation of Feynman diagrams in several large packages (both numerical and symbolic computations) [23–27].

The program complex operates in a batch mode fully. The program accepts the file with model description in the form of interaction equation (equations of chemical kinetics). The output is a set of model equations and Feynman diagrams [28] needed for basic kinetic equation solution.

The model equations are obtained by the developed technique [6, 7, 29, 30]. On the basis of interaction equation the intensities of forward and backward transitions are calculated. From the expressions for the intensities three types of model equations are constructed: the master equation, the Fokker–Planck equation, the stochastic differential equation in the Langevin form. This fragment of program complex is internally completed, because of the independent research may be carried out based on the obtained model equations.

Then the solution of master equation is obtained. For this purpose, the Liouville operator is constructed with the help of some presented in the work substitutions. On the basis of Liouville operator Feynman diagrams are derived [31–33].

7. Conclusions

Thus, the proposed program complex consists of two principal parts. The first part implements the methodology of one-step processes stochastization. A structure for the master equation solution within the operator perturbation theory approach is realised by the second part.

It seems that the given approach will to be extremely productive in solution of population dynamics problems, epidemiological models, models of network protocols and telecommunication systems. However, the proposed approach is not limited within one-step models. Its extension to other stochastic processes is quite possible.

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Квантово-полевой подход к анализу одношаговых моделей

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При разработке методики стохастизации одношаговых процессов основное внимание было уделено получению стохастических уравнений в форме Ланжевена, поскольку данный вид наиболее привычен при построении и исследовании данного круга моделей. Но в ходе применения метода возникает проблема обоснования перехода от основного кинетического уравнения к уравнению Фоккера–Планка для разных вариантов модели. При этом формы уравнений в частных производных (основное кинетическое уравнение и уравнение Фоккера–Планка) могут предоставить исследователю более богатое описание модели. Для обоснования возможности разложения основного кинетического уравнения и для исследования модельных уравнений предлагается использовать теорию возмущений в форме, реализованной в рамках квантовой теории поля. Для этого описана методика и создан аналитический программный комплекс приведения основного кинетического уравнения к операторной форме в фоковском представлении. Для решения получившегося уравнения в рамках программного комплекса проводится генерация фейнмановских диаграмм для соответствующего порядка теории возмущений. В качестве системы символьных вычислений была применена система FORM. Выбор FORM обоснован тем, что данная система компьютерной алгебры позволяет проводить символьные вычисления, используя ресурсы высокопроизводительной вычислительной техники. В частности, возможно использовать такие технологии параллельных вычислений, как OpenMP и MPI.

Ключевые слова: символьные методы в биологии: стохастические дифференциальные уравнения; основное кинетическое уравнения; уравнение Фоккера–Планка; популяционные модели; системы компьютерной алгебры; система FORM.

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