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PHYSICAL FOUNDATIONS OF MATHEMATICAL MODELING

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Abstract

This article is an introduction to mathematical modeling of real world processes and of complex systems. It is devoted to the development of the description of dynamical systems in terms of statistical physics. Such a description provides a necessary “bridge” between the dynamical properties of a system and its treatment in terms of macroscopic quantities, involved in mathematical model, i.e. in terms of statistical quantities.

1. Statistical description of dynamical systems

We will deal with mathematical models of the systems that possess certain dynamics. The system can be very complicated and not of pure mechanical nature. But we will assume that there exist a set of “dynamical” variables $x = (x_1, x_2, .., x_n)$ that obey the equation of motion:

$$\dot{x}_i = f_i(x,t), \; i = 1,2,...,n \; , \tag{1.1}$$

Where f_i are given functions of x_k (k = 1, 2, …, n) and time t. Solving the systems of the equations (1.1) together with initial conditions:

$$x_i(t)\big|_{t=0} = x_i(0) = x_{i_0} \; , \tag{1.2}$$

We get a complete of total description of the system under consideration:

$$x_i(t) = x_i(x(0),t) \; . \tag{1.3}$$

We will use the term “model” description in two senses – wide and narrow. In a wide sense every description of a real system has a model character. But when this description is based on the dynamical approach (1.1)-(1.2), we will call it “exact” or “complete” description. Usually the dynamical approach is very complicated and practically can’t be realized. In this case we try to get some simplified reduced description of a system under consideration and call it to be a “model” description in a narrow sense. We will see that principal existence of the dynamics (1.1)-(1.2) leads to certain restrictions of the form in which the reduced model description can be presented, even in the cases when this “exact” dynamics is not known in an explicit form.

In the case of classical mechanical systems the complete set of dynamical variables consists of coordinate $\{q_i\}$ and momentum $\{p_i\}$ sets, which satisfy the Hamiltonian equations:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}; \quad \dot{p}_i = -\frac{\partial H}{\partial q_i} \ , \tag{1.4}$$

where $H(q_1,...,q_n,p_1,...,p_n,t)$ is the Hamiltonian function of the system. Analogous considerations can be developed for quantum systems, but for the sake of simplicity we will deal here with classical systems. In the case of more complicated systems (biological, chemical, etc.) the dynamics can be of non-Hamiltonian type. In these cases we will deal with the systems of equations (1.1)-(1.2).

Main principles of developing of mathematical models of the systems that possess dynamics in the sense (1.1)-(1.2) can be established on the basis of modern statistical physics with its fundamental rules of the transition to reduced description.

First of all, let us represent the dynamical problem (1.1)-(1.2), that leads to exact description (1.3), in terms of statistical physics. In statistical physics we deal with mean values $\langle A \rangle$ of different physical quantities *A*. These mean values are obtained with the help of distribution function $\rho(x,t)$:

$$\langle A \rangle = \int dx \, \rho(x,t) A(x,t) \ . \tag{1.5}$$

Integration in (1.5) is performed over complete set of dynamical variables:

$$dx = dx_1 ... dx_n \ . \tag{1.6}$$

The distribution function $\rho(x,t)$ is a subject to normalization condition:

$$\int dx\,\rho(x,t) = 1 \ . \tag{1.7}$$

It is easy to see that if we choose the dynamical distribution function $\rho_d(x,t)$ in the form:

$$\rho_d(x,t) = \delta\big(x - x(t)\big) \ , \tag{1.8}$$

where $\delta\big(x - x(t)\big)$ is the Dirac delta-function:

$$\delta\big(x - x(t)\big) = \delta\big(x_1 - x_1(t)\big)...\delta\big(x_n - x_n(t)\big) \ , \tag{1.9}$$

then mean values of any physical quantity $\langle A \rangle$ will coincide with their instant values $A(t)$ at the moment *t*:

$$\langle A \rangle = \int dx\,\delta\big(x - x(t)\big)A(x,t) = A(x(t),t) \equiv A(t) \ . \tag{1.10}$$

We would like to emphasize that *x* here denotes a dynamical variable, and $x(t)$ is a function of time *t* given by (1.3).

Statistical distribution function $\rho(x,t)$ can be obtained by means of averaging of the dynamical distribution function $\rho_d(x,t)$ over all possible values of initial conditions $x(0)$:

$$\rho(x,t) = \int dx(0)\,\delta\big(x - x(t)\big)\rho_0(x(0),0) \ , \tag{1.11}$$

where $\rho_0(x(0),0)$ is a distribution function (obtained with the help of some physical considerations) at the initial time $t = 0$.

It can be proved that the distribution function $\rho(x,t)$ will satisfy the normalization condition (1.7) at any moment of time, if $\rho_0(x(0),0)$ satisfies the condition:

$$\int dx(0)\,\rho_0(x(0),0) = 1 \ . \tag{1.12}$$

Indeed, we get with the help of (1.11) and (1.12):

$$\int dx\rho(x,t) = \int dxdx(0)\,\delta\big(x - x(t)\big)\rho_0(x(0),0) = \int dx(0)\,\rho_0(x(0),0) = 1 \ .$$

If a real system under consideration obeys the Hamiltonian dynamics, then its statistical distribution function satisfies the Liouville equation:

$$\frac{\partial \rho}{\partial t} + [H, \rho] = 0 \ , \tag{1.13}$$

where H is a Hamiltonian function, and $[H, \rho]$ is a classical Poisson brackets:

$$[H, \rho] = \sum_{i=1}^{N} \left(\frac{\partial \rho}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial q_i} \right) . \tag{1.14}$$

Here N is a number of degrees of freedom, which is equal to $n/2$, where n are a total number of dynamical variables.

If the dynamics of the system is not of Hamiltonian type, then the equation of evolution for its statistical distribution function can be obtained in the following way. We differentiate the expression (1.11) with respect to time t using a chain rule:

$$\frac{\partial \rho(x,t)}{\partial t} = -\sum_{i=1}^{N} \int dx(0) \ \frac{\partial}{\partial x_i} \delta\left(x - x(t) \right) \dot{x}_i(t) \rho_0(x(0), 0) \, . \tag{1.15}$$

Partial derivatives $\frac{\partial}{\partial x_i}$ can be taken out of the integrand; the quantities $\dot{x}_i(t)$ can be changed for $f_i(x,t)$ according to (1.1) due to the fact that the integrand contains delta-function. Thus, we get:

$$\frac{\partial \rho(x,t)}{\partial t} = -\sum_{i=1}^{N} \frac{\partial}{\partial x_i} \int dx(0) \ \delta\left(x - x(t) \right) \rho_0(x(0), 0) \cdot f_i(x,t) \, . \tag{1.16}$$

Taking into account the definition (1.11) of a statistical distribution function, we finally get:

$$\frac{\partial \rho(x,t)}{\partial t} + \sum_{i=1}^{N} \frac{\partial}{\partial x_i} \left\{ \rho(x,t) \, f_i(x,t) \right\} = 0 \ . \tag{1.17}$$

It is easy to check, that in the case of Hamiltonian systems, when $x = \{q_i, p_i\}$ with the equations of motions (1.4), the equation of evolution of a distribution function (1.17) turns to be a Liouville equation (1.13).

The equation (1.17) has a sense of continuity equation. If we recollect that the functions $f_i(x,t)$, according to the equation (1.1), correspond to "velocities" $\dot{x}_i$ of the quantities x_i, then it becomes clear that this equation has a form:

$$\frac{\partial\rho(x,t)}{\partial t}+\operatorname{div}\left(\rho(x,t)\vec{v}(x,t)\right)=0 \ , \tag{1.18}$$

where $\vec{v}$ is a vector in *n*-dimensional space with the components.

$$\vec{v}=\left(f_1(x,t), f_2(x,t),..., f_n(x,t)\right) \ , \tag{1.19}$$

and div means the divergence in *n*-dimensional space. This is a quite expectable result if we take into account the condition (1.7).

Mean values $\langle A\rangle$ of the quantities *A*, determined with the help of (1.5), possess on useful property:

$$\left\langle\frac{dA}{dt}\right\rangle=\frac{d}{dt}\langle A\rangle \ . \tag{1.20}$$

To prove this property, let us substitute the definition (1.11) into the expression (1.5):

$$\langle A\rangle=\int dxdx(0)\delta\left(x-x(t)\right)\rho_0(x(0),0)A(x,t) \ . \tag{1.21}$$

Changing the order of integration in (1.21), we get:

$$\langle A\rangle=\int dx(0)\rho_0(x(0),0)A(x(t),t) \ . \tag{1.22}$$

Comparing the expressions (1.5) and (1.22) we observe, that averaging of the quantity $A(x,t)$ at the moment of *t* can be produced either with the help of distribution function $\rho(x,t)$ taken at the same moment *t* (exp. (1.5)), or with the help of the initial distribution function $\rho_0(x(0),0)$, but in this case, according to (1.22), we need to know the time-dependence of $x(t)$, i.e. need the solution (1.3) of the dynamical equations. Now, if we look for $\left\langle\frac{dA}{dt}\right\rangle$, then, according to (1.22), we can write:

$$\left\langle\frac{dA}{dt}\right\rangle=\int dx(0)\rho_0(x(0),0)\frac{dA\left(x(t),t\right)}{dt} \ . \tag{1.23}$$

But exactly the same expression will be obtained if we differentiate (1.22) with respect to time:

$$\frac{d}{dt}\langle A\rangle=\int dx(0)\,\rho_0(x(0),0)\frac{dA\big(x(t),t\big)}{dt}\ . \qquad (1.24)$$

Comparison of (1.23) and (1.24) proves the validity of (1.20).

2. The reduced description of complex dynamical systems

The usual intuitive approach to the reduced description of complex systems can be verified by mans of the method of projection operators. Let us assume that the complete description of the system under consideration can be described on the basis of partial differential equation:

$$\frac{\partial\rho}{\partial t}+iL\rho=0\ , \qquad (2.1)$$

where ρ the complete distribution function, and L is is some operator that determines the “dynamics” of the system. For example, for classical mechanical system equation (2.1) is a Liouville equation, and L is a Liouville operator:

$$L=-i\sum_{i=1}^{N}\left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i}-\frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i}\right)\ , \qquad (2.2)$$

where the sum is performed over all degrees of freedom of the system. To determine the behavior of the system we are to solve the Cauchy problem for the given initial distribution $\rho(0)=\rho(t)\big|_{t=0}$.

We consider that there exists a projection operator P that assigns the reduced distribution function $\rho_1(t)$:

$$\rho_1(t)=P\rho(t)\ . \qquad (2.3)$$

Now we introduce the function $\rho_2(t)$ by the equation:

$$\rho_2(t)=(1-P)\rho(t)\ , \qquad (2.4)$$

so that

$$\rho_1(t)+\rho_2(t)=\rho(t)\ . \qquad (2.5)$$

The equations for the functions $\rho_1(t)$ and $\rho_2(t)$ are easily obtained with the help of the equation (2.1):

$$i\frac{\partial \rho_1}{\partial t} = PL(\rho_1 + \rho_2) \;; \tag{2.6}$$

$$i\frac{\partial \rho_2}{\partial t} = (1-P)L(\rho_1 + \rho_2) \;. \tag{2.7}$$

We write the equation (2.7) in the form:

$$i\frac{\partial \rho_2}{\partial t} = M\rho_2 + \varphi(t) \;, \tag{2.8}$$

where the operator M and the function φ are defined as:

$$M = (1-P)L \;; \tag{2.9}$$

$$\varphi(t) = (1-P)L\rho_1 \;. \tag{2.10}$$

We look for the normal solution of the equation (2.8) in the form:

$$\rho_2(t) = \mathrm{e}^{-itM}\psi(t) \;, \tag{2.11}$$

where operator M is determined by the equation (2.9). Now the equation (8) reads:

$$\frac{\partial \psi}{\partial t} = -i\mathrm{e}^{itM}\varphi(t) \;, \tag{2.12}$$

with the initial condition written in the form:

$$\psi(0) = \rho_2(0) \;. \tag{2.13}$$

Integrating the equation (2.12) with respect to time t over the limits 0, t, we get:

$$\psi(t) = \psi(0) - i\int_0^t d\tau\, \mathrm{e}^{i\tau M}\varphi(\tau) \;. \tag{2.14}$$

Now we substitute the expression (2.14) to the formula (2.11) to get:

$$\rho_2(t) = \mathrm{e}^{-itM}\rho_2(0) - i\int_0^t d\tau\, \mathrm{e}^{-i(t-\tau)M}\varphi(\tau) \;. \tag{2.15}$$

Changing the variable $s = t - \tau$, we obtain:

$$\rho_2(t) = \mathrm{e}^{-itM}\rho_2(0) - i\int_0^t ds\,\mathrm{e}^{-isM}\varphi(t-s) \ . \tag{2.16}$$

Or, with the explicit expressions (2.9) and (2.10) for M and $\varphi(t)$:

$$\rho_2(t) = \exp\big(-it(1-P)L\big)\rho_2(0) - i\int_0^t ds\exp\big(-is(1-P)L\big)\cdot(1-P)L\rho_1(t-s) \ . \tag{2.17}$$

Finally, substituting (2.17) into (2.6), we get the equation for $\rho_1(t)$, which can be called "master" equation:

$$\begin{aligned} i\frac{\partial\rho_1}{\partial t} &= PL\rho_1(t) + PL\exp\big(-it(1-P)L\big)\rho_2(0) - \\ &-i\int_0^t ds\,PL\exp\big(-is(1-P)L\big)\cdot(1-P)L\rho_1(t-s) \ . \end{aligned} \tag{2.18}$$

Equation (2.18) is an exact equation, equivalent to the initial equation (2.1) (together with the equation (2.17) for $\rho_2(t)$). No any approximations were used during the derivation of (2.18). But now the equation (2.18) for the reduced distribution function $\rho_1(t)$ is a delay equation; it has a non-local character in time: the system is assumed to possess a "memory". In order to get a closed equation for $\rho_1(t)$ we are to exclude or set in an explicit form the value of $\rho_2(0)$. Relaxation time τ essentially appears in such approach and verifies the intuitive reduction of the description of the system. In practice, we don't know the complete dynamics of a complex system and can't introduce the equation (2.1) in the explicit form. The necessity of phenomenological approach to the theory of complex systems of arbitrary nature becomes evident and the most general form of the master equation for the reduced description is established provided the system possess the complete dynamics (although unknown by us). At the same time some conclusions concerning the properties of the kernel in the equation (2.18) can be made on the basis of truthful physical (biological, etc, …) considerations. A more difficult problem is to prescribe the initial condition for $\rho_2(0)$, if it is introduced in an explicit form: we must not involve contradictions between the second and the third terms in the right side if the equation (2.18).

The existence of "memory" is a well-known fact in any phenomenological description of macroscopic properties of real physical systems. This phenomenon is easily accepted in the intuitive construction of the models of complex systems even in the cases when the systems do not posses a certain dynamics. Now this idea received a rigorous verification on the basis of a strict dynamical approach to the theory of real systems.