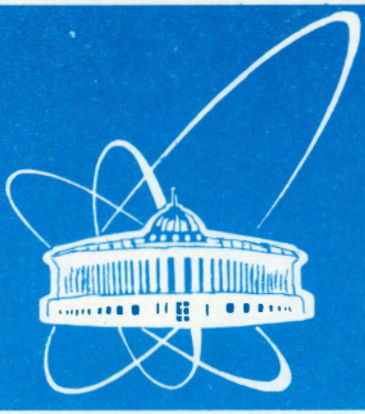

СООБЩЕНИЯ
ОБЪЕДИНЕННОГО
ИНСТИТУТА
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

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THE CORRESPONDENCE BETWEEN CHEMICAL SCHEMES AND DYNAMICAL LOTKA—VOLTERRA SYSTEMS

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1. Introduction

It is known that Lotka-Volterra systems (LVS) of Ordinary first-order Differential Equations (ODE) are applied to describe some kinds of nonlinear interactions in various branches of science. Historically, LVS appeared to model interactions between interconnective biological species [1, 2], and to study kinetics of chemical reactions [2]. Later, LVS have aroused considerable interest due to problems of the mode coupling of waves in physics of lasers [3]. Interest in LVS was revived by the paper [4]. It was established there that the fine structure of spectra of Langmuir waves in plasma is described through a special VS with all the coefficients being equal to ± 1. The next step was made by L.Brenig. He proved [5] that a large set of ODE's (the so-called generalized LVE) implied in various fields of physics, biology, chemistry, and economics, can be reduced to LVE by quasimonomial transformations of the variables. Korzukhin, as has been reported in the book by Ebeling [6], proved the following theorem:
if

$$dC_i/dT = F_i(C_1, C_2, ..., C_f), \quad i = 1, 2, ..., f,$$

where C_i is the concentration of the i-th reagent and F_i is an arbitrary polynomial of non-negative integer power,
it is possible to build at least one asymptotically equivalent chemical reacting system.
Thus, due to this fact, arbitrary nonlinearities are permissible within the chemical kinetics.

The formal reacting system by Lotka [2] is written as a system of chemical arrow equations

$$\begin{array}{ccc} A + X_1 & \xrightarrow{k_1} & 2X_1, \\ X_1 + X_2 & \xrightarrow{k_2} & 2X_2, \\ X_2 & \xrightarrow{k_3} & F \end{array} \qquad (1)$$

and is described through Lotka's system of ODE

$$\begin{array}{rcl} \dot{X}_1 & = & AX_1 - AX_1X_2, \\ \dot{X}_2 & = & X_1X_2 - X_2. \end{array} \qquad (2)$$

where $X_1 = C_1k_2/k_3$, $X_2 = C_2k_2/k_3$, $A = k_1C_A/k_3$, $\tau = k_3t$. It must be remarked that this form of equations can be written under the assumption C_A (a concentration of A) = const.

Now we consider the three-component system of ODE

$$\begin{array}{rcl} \dot{x}_1 & = & \alpha x_1x_3 - \gamma x_1x_2, \\ \dot{x}_2 & = & \beta x_2x_3 + \gamma x_1x_2, \\ \dot{x}_3 & = & -\alpha x_1x_3 - \beta x_2x_3. \end{array} \qquad (3)$$

The system (3) is a special form of VS, which was introduced in our papers [7, 8]. Solutions and a detail investigations of (3) are given in our papers [8, 9, 10]. The peculiarity of (3) is the skew-symmetric matrix of coefficients. As a result, diagonal terms are equal to zero and that is why terms proportional to X_iX_i are absent. Besides, there are no linear terms in the system (3). It means, from the chemical or formal kinetics point of view, that the left-hand side of appropriate arrow equations cannot contain terms like $2X$, where X labels an arbitrary chemical substance. For example, the reaction $2S \to T + ...$ stipulates in the corresponding differential equation a term proportional to C_S^2, where S and T are substances and C_S is a concentration of S in the common chemical notation.

Let us notice, that VS is a subcase of equations LVS [1]

$$\dot{x}_i = x_iy_i, \quad i = 1, ..., N; \quad where\ y = Ax + b \qquad (4)$$

if there exist such $\beta_i \neq 0$, that $\beta_ia_{ij} = -\beta_ja_{ji}$, but system (3) is its subcase ($\beta_i = 1, i = 1, ..., N; b = 0$). Moreover, in turn, system (3) is the general case of VS with antisymmetric interaction matrix (see [9, 10]).

We attempt to find some example of a chemical system that is described with in those differential equations.

2. Conversion of formal kinetic

The formal kinetics point of view is that an actual chemical process 1) is described by a set of chemical equation formulae approximately which in its turn that 2) produces a set of ordinary differential equations. After solving these equations one can study some of their properties and of real chemical reaction, if he is lucky.

The reverse way to deal with this problem is to obtain a set of chemical equation formulae for a given set of differential equations, so that the kinetic properties of a real chemical process are described in terms of the properties of solutions of those differential equations.

One can say it is not important, if there are no chemical equation exactly for these differential equations because real chemical phenomena are described by the known formalism of chemical equations only approximately. But from a theoretical point of view it is very important to know that no finite set of chemical equations will be sufficient what ever detailed the description of the processes treat may not be (but in the same formalism).

We cannot give a regular rule how to get a chemical equation from the differential one. But if we can enumerate all sets of chemical equations in some formal language (maybe some of the mentioned sets of equations can be found meaningless but later on this will not lead to consequences), we hope that it will be found in the course of enumeration if a suitable answer exists (using the direct kinetics correspondence rule to verify it). So, one needs now only to formulate the exact definition of this enumerable formal class.

3. Class definition

Let us consider the class K of dynamical systems

$$D = (A_D, P_D, Q_D),$$

where $A_D = \{A_1, A_2, ...\}$ is an alphabet, that is, the finite list of "chemical substances" and variables of the same names,

$P_D = \{P_1, P_2, ...\}$ is the finite list of schemes of "chemical reactions" of the form

$$P_i : \alpha_{i1}A_1 + \alpha_{i2}A_2 + ... \xrightarrow{k_i} \beta_{i1}A_1 + \beta_{i2}A_2 + ..., \qquad (5)$$

where all α_{ij}, β_{ij}, k_i are different symbols.

$Q_D = \{Q_1, Q_2, ...\}$ is the list of ODE in the one-to-one correspondence to each variable of the alphabet A_D of the form

$$Q_j : dA_j/dt = \sum_{P_i \in P_D} k_i(\beta_{ji} - \alpha_{ji}) \prod_{A_k \in A_D} A_k^{\alpha_{ki}}. \qquad (6)$$

Any set of "formal chemical equations" may be found as a member of that class and vice versa: some set of differential equations may be found there. The equations are considered equal to each other if they are identical after substitution of some numbers or expressions instead of symbols α_{ij}, β_{ij}, k_i.

Now one can formulate any problems, concerning the existence (or nonexistence) of some schemes, so that the predefined ODE satisfy them or may be converted into those.

4. The problem

The problem is the existence of a system D in the class K, such that its component Q_D has the form

$$\begin{aligned} \dot{x} &= \alpha xz - \gamma xy, \\ \dot{y} &= \beta yz + \gamma yx, \\ \dot{z} &= -\alpha zx - \beta zy. \end{aligned} \qquad (7)$$

5. Solution

In general, the problem stated may be unresolved or resolved in negative sense. But this problem has a simple solution

$$\begin{aligned} x + y &\xrightarrow{k_1} 2y, \\ y + z &\xrightarrow{k_2} 2z, \\ z + x &\xrightarrow{k_3} 2x, \end{aligned} \qquad (8)$$

where $k_1 = \gamma, k_2 = -\beta, k_3 = \alpha$.

6. Growth and disintegration

The well - known case is

$$\begin{aligned} A_D &= \{x\}, \\ P_D &= \{P_x : \alpha x \xrightarrow{k} \beta x\}, \\ Q_D &= \{Q_x : \dot{x} = k(\beta - \alpha)x^\alpha\}. \end{aligned} \qquad (9)$$

If $k(\beta - \alpha) > 0$ it corresponds to growth; otherwise, to disintegration.

A more general equation

$$\dot{x} = f(y), \text{ with being of continuous } f(y) \neq 0 \qquad (10)$$

is of the same kind due to the conversion

$$x = e^{\int \frac{dy}{f(y)}}, \text{ and } k(\beta - \alpha) = 1. \qquad (11)$$

Let us treat the case

$$A_D = \{x\}.$$
$$P_D = \left\{ \begin{array}{l} \mathrm{P}_1 : \alpha_1 x \xrightarrow{k_1} \beta_1 x \\ \ldots \\ \mathrm{P}_n : \alpha_n x \xrightarrow{k_n} \beta_n x \end{array} \right\}. \qquad (12)$$
$$Q_D = \{\mathrm{Q}_x : \dot{x} = \textstyle\sum_{i=1}^{n} k_i(\beta_i - \alpha_i)x^{\alpha_i}\}$$

for some simultaneous processes of growth and disintegration.

The system (12) may have some critical points (where the right part of ODE equals to 0), i.e. stable, equilibrium points of the kind of a focus. No other kind of critical points exists in one-dimensional case.

Any equation of the type

$$\dot{y} = f(y),$$

whose finite set of critical points (where $f(y) = 0$) equals a set of zeroes

$$\textstyle\sum_{i=1}^{n} k_i(\beta_i - \alpha_i)x^{\alpha_i} = 0,$$

is of the same kind as (12) due to the conversion satisfying the equation

$$\frac{dx}{\sum_{i=1}^{n} k_i(\beta_i - \alpha_i)x^{\alpha_i}} = \frac{dy}{f(y)}.$$

7. Case of two substances

Let us treat the case

$$A_D = \{x, y\},$$
$$P_D = \{\mathrm{P} : \alpha_1 x + \alpha_2 y \xrightarrow{k} \beta_1 x + \beta_2 y\},$$
$$Q_D = \left\{ \begin{array}{l} \mathrm{Q}_x : \dot{x} = k(\beta_1 - \alpha_1)x^{\alpha_1} y^{\alpha_2}, \\ \mathrm{Q}_y : \dot{y} = k(\beta_2 - \alpha_2)x^{\alpha_1} y^{\alpha_2} \end{array} \right\}. \qquad (13)$$

It is easily seen that the integral curves of those ODE are

$$y = \frac{\beta_2 - \alpha_2}{\beta_1 - \alpha_1} x + C,$$

where C is an arbitrary constant.

The set of critical points of ODE include the union of coordinate axes ($x = 0$ *or* $y = 0$).

8. Linear ODE's

Let us consider such a subclass of the class of dynamical systems, which has α_{ij} in (5) all equal to 0 or 1 only but only one coefficient α_{ij} equal to 1 for each equation $\mathrm{P_i}$.

It is well known case of linear ODE's. All sets of critical points in that case are linear subspaces.

9. Quadratic ODE's

Let us consider such a subclass of the class of dynamical systems, which has α_{ij} in (5) all equal to 0 or 1 only but no more than two coefficients α_{ij} equal to 1 for each equation $\mathrm{P_i}$.

It is the case of Lotka-Volterra systems (LVS). The reason for such a constrain is that known correct kinetic processes have chemical equations, which may contain one, two or three substances in their left-hand side. In other cases those equations must be detailed with the aid of intermediate substances.

10. Qualitative kinetical consideration. Examples

As is known, formal reactions are usually written in the form

$$\mathrm{P_i} : \alpha_{i1}A_1 + \alpha_{i2}A_2 + \ldots \underset{k_{2i}}{\overset{k_{1i}}{\rightleftharpoons}} \beta_{i1}A_1 + \beta_{i2}A_2 + \ldots, \qquad (14)$$

where both the arrows have their $k_1, k_2 > 0$. It is a restriction on the original class of dynamical systems and the problem defined may be unsolvable.

In a formal kinetical context this is meant that reactions are interpreted as reversible quasistationary ones. Really, at each given instant both the direct and reverse reactions occur. This difference between reactions mentioned above leads to a certain direction of the course of reaction until the point of equilibrium is reached. Let us suggest existence of some correspondence between equations (8) and certain real chemical reactions. In that case we can say, that those reactions can be described only in the limit of $k_{2i} \to 0$ (see eq. (14)). In other words, they must be asymptotically non-reversible.

In the case of quark physics the above scheme of reasoning may be applied too. Let us now consider a "quark" gase composed of three subsystems with equal numbers of quarks coloured in, say, blue (b), green (g) and yellow (y) colours, which is confined within a closed bag. At equal proportions of colours the system as a whole we shall assume to be colourless. Let us call collisions of quarks of the same colour elastic collisions, and collisions of quarks of different colours–inelastic. Further, let us define the following rule of colours transfer: a blue quark changes its colour to green after a collision with a green one, a green quark–to yellow after a collision with a yellow one, and a yellow quark becomes blue after a collision with a blue one, i.e.

$$b+g \to g+g, \quad g+y \to y+y, \quad y+b \to b+b. \tag{15}$$

Given this rule of colour transmission, when there are three quarks only in the bag any *random* choice of the first collision to take place inevitably leads to a causal chain of the processes (16), resulting in the coloured final state.Indeed,

$$b+g \to g+g, \quad g+y \to y+y, \quad g+y \to y+y, \tag{16}$$

which corresponds to the following chain of changes of internal states inside the bag: $bgy \to ggy \to gyy \to yyy$. Thus, the last quark to enter "the game" is the one to "win", because his antagonist is lost in the "first combat".

When in our "hadron" the number of quarks of each colour is "very large" (that correspond to the current quarks representation in the quark theory) and all three inelastic reactions run with the same intensity, then the object can be regarded as colourless during periods of time that are greater than the mean time of collision. Suppose now, that the object is absolutely stable, so that we can't fix the fluctuations of its colour by means of measuring random painting of its decay products statistics. Then we can, on the same basis, construct a model without any elastic or inelastic collisions within the bag. In other words ,if the reactions within a compound system form a closed cycle, then statistical equilibrium cannot be distinguished from the absence of dynamical microscopic interactions.

The most part of the solutions of eqs (3) describes the statistical equilibrium in a system of three isolated phases. That is why we cannot take initial conditions with one of the phases absent in order to achieve an "equilibrium" solution, and the system, in "quark" terms, inevitably acquires one of the two remaining colours.

It should be pointed out, that the aperiodic solutions of the system (3) posesses, by the following remarkable property. Namely, this is the drift of representative point on the phase triangle into any of its corners where in the very vertex any two of three phases disappear (that correspond to colouring of the object in consideration). This state occurs in infinite period of time.

In the physics of real quarks such a situation is impossible due to an additional condition: the exclusion principle for fermions which prohibits the presence of two quarks with the same colour (and the same other quantum numbers) within a common well (a given hadron), i.e. in the field of action of their generalized mean potential. Moreover, the essential point in our context is that the quark–gluon quantum field theory forbids the quark-quark interactions at small distances in general. which is called the asymptotical ultraviolet freedom of quark.

11. Conclusion

It is shown in this paper that the Lotka-Volterra-kind system of ODE stipulates a formal chemical-kinetics system written down in a usual formalism of arrow equations. On an assumption of existence of some correspondence between equations (8) and certain real chemical reactions we can say that those reactions can be described only in the limit of $k_{2i} \to 0$ (see eq. (14)) and, in other words, they must be asymptotically non-reversible.

We discuss a possible interpretation of the mathematical object (3) as a (multi)quark colourless one consisting of three painted interacting species of quarks. The system (3) has a special form of VS, which was introduced in our papers [7, 8]. The peculiarity of (3) is the skew-symmetric matrix of coefficients. Solutions and detailed investigations of (3) are given in papers [8, 9, 10]. But now we realize that a classification of solutions eq. (3) must be done as a whole. It will be given in the next paper.

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Соответствие между химическими схемами и динамическими системами Лотка—Вольтерра

Показано, что система ОДУ типа Лотка—Вольтерра

$$\dot{x} = \alpha xz - \gamma xy,\ \ \dot{y} = \beta yz + \gamma yx,\ \ \dot{z} = -\alpha zx - \beta zy \qquad (1)$$

обуславливает некоторую формально-кинетическую систему в формализме стрелочных уравнений, имеющую вид

$$x + y \xrightarrow{k_1} 2y,\ \ y + z \xrightarrow{k_2} 2z,\ \ z + x \xrightarrow{k_3} 2x, \qquad (2)$$

где $k_1 = \gamma$, $k_2 = -\beta$, $k_3 = \alpha$. Пара из системы ОДУ и системы стрелочных уравнений принадлежит введенному в работе классу динамических систем, определяемых алфавитом перемеиных состояния и законами движения, записанными в формализмах как стрелочных (AE), так и дифференциальных (ODE) уравнений в виде соответствующих списков. Обсуждается возможность интерпретации математического объекта (1) как «многокваркового» белого (бесцветного), состоящего из трех сортов окрашенных взаимодействующих кварков, причем таким образом, что их перманентное трехчастичное взаимодействие не распадается на двухчастичные в силу антисимметричности матрицы взаимодействия.

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The Correspondence between Chemical Schemes and Dynamical Lotka—Volterra Systems

It is shown that the Lotka—Volterra-kind system of ODE

$$\dot{x} = \alpha xz - \gamma xy,\ \ \dot{y} = \beta yz + \gamma yx,\ \ \dot{z} = -\alpha zx - \beta zy \qquad (1)$$

stipulates a formal chemical-kinetics system written down in a usual formalism of arrow equations as

$$x + y \xrightarrow{k_1} 2y,\ \ y + z \xrightarrow{k_2} 2z,\ \ z + x \xrightarrow{k_3} 2x, \qquad (2)$$

where $k_1 = \gamma$, $k_2 = -\beta$, $k_3 = \alpha$. A couple of systems of ODE's and arrow equations belong to the class K of dynamical systems $D = (A_D, P_D, Q_D)$ introduced in the present paper, i.e. dynamical systems that are defined through their variables of state (so-called alphabet A_D) and laws of motion written down both in the arrow equation (AE) formalism (a list of AE P_D), and the ODE one (a list of corresponding ODE's Q_D). The problem is the existence of such a system D in the class K that its components Q_D could be written down as AE's. The correspondence between equations (1) and (2) give a simple solution of the problem. We discuss a possible interpretation of the mathematical object (1) as a (multi) quark colourless one consisting of three painted interacting species of quarks.

The investigation has been performed at the Laboratory of High Energies, at the Bogoliubov Laboratory of Theoretical Physics, at the Laboratory of Computing Techniques and Automation, JINR.

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