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КОМПЬЮТЕРНЫЕ ТЕХНОЛОГИИ В ФИЗИКЕ

DISCRETE SYMMETRY ANALYSIS OF LATTICE SYSTEMS

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Discrete dynamical systems and mesoscopic lattice models are considered from the point of view of their symmetry groups. Some peculiarities in behavior of discrete systems induced by symmetries are pointed out. We reveal also the group origin of moving soliton-like structures similar to *spaceships* in cellular automata.

Дискретные динамические системы и мезоскопические решеточные модели рассматриваются с точки зрения их групп симметрий. Указаны особенности поведения дискретных систем, обусловленные наличием нетривиальных симметрий. Выявлена групповая природа солитоноподобных движущихся структур типа *космических кораблей* в клеточных автоматах.

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INTRODUCTION

There are many philosophical and physical arguments that discreteness is more suitable for describing physics at small distances than continuity which arises only as a logical limit in considering large collections of discrete structures.

Recently [1, 2] we showed that any relation on collection of discrete points taking values in finite sets naturally has a structure of *abstract simplicial complex* — one of the mathematical abstractions of locality. We call such collections *discrete relations on abstract simplicial complexes*. Special cases of this construction are, e.g., systems of *polynomial equations* over finite fields and *cellular automata*.

Here we study symmetry properties of discrete dynamical systems on graphs — one-dimensional simplicial complexes. The study is based essentially on our C program for symmetry analysis of discrete systems. The program, among other things, constructs and investigates *phase portraits* of discrete dynamical systems *modulo groups* of their symmetries, searches dynamical systems possessing specific properties, e.g., *reversibility*, computes microcanonical *partition functions* and searches *phase transitions* in mesoscopic systems. Some computational results and observations are presented. In particular, we explain formation of moving soliton-like structures similar to *spaceships* in cellular automata.

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1. LATTICES, FUNCTIONS AND SYMMETRIES

Lattices. Traditionally, the word «lattice» is applied to some regular system of separated points of a continuous metric space. In many problems of applied mathematics and mathematical physics neither metrical relations between discrete points nor existence of underlying continuous manifold do matter. The notion of «adjacency» for pairs of points is essential only. All problems considered in the paper are of this kind. Thus, we define here a *lattice* as indirected k-regular graph Γ without loops and multiple edges whose *automorphism group* $\mathrm{Aut}\,(\Gamma)$ acts transitively on the set of vertices $V(\Gamma)$.

Computing Automorphisms. The automorphism group of graph with n vertices may have up to $n!$ elements. However, McKay's algorithm [3] determines this group by constructing small number (not more than $n-1$, but usually much less) of the generators.

In Sec. 2 we consider concrete example of system on square lattice in order to explain the formation of soliton-like structures in discrete systems. So let us describe symmetries of $N \times N$ square lattices in more detail. We assume that the lattice has valency 4 («von Neumann neighborhood») or 8 («Moore neighborhood»). We assume also that the lattice is closed into discrete torus $\mathbb{Z}_N \times \mathbb{Z}_N$, if $N < \infty$. Otherwise, the lattice is discrete plane $\mathbb{Z} \times \mathbb{Z}$. In both von Neumann and Moore cases the symmetry group, which we denote by $G_{N\times N}$, is the same. The group has the structure of *semidirect* product of the subgroup of *translations* $\mathbf{T}^2 = \mathbb{Z}_N \times \mathbb{Z}_N$ (we assume $\mathbb{Z}_\infty = \mathbb{Z}$) and *dihedral group* $\mathbf{D}_4$

$$G_{N\times N} = \mathbf{T}^2 \rtimes \mathbf{D}_4, \quad \text{if} \quad N = 3, 5, 6, \ldots, \infty. \tag{1}$$

The dihedral group $\mathbf{D}_4$ is the semidirect product $\mathbf{D}_4 = \mathbb{Z}_4 \rtimes \mathbb{Z}_2$. Here $\mathbb{Z}_4$ is generated by 90° rotation, and $\mathbb{Z}_2$ is reflections. The size of $G_{N\times N}$ is $|G_{N\times N}| = 8N^2$, if $N \neq 4$. In the case $N = 4$ the size of the group becomes three times larger than expected $|G_{4\times 4}| = 3 \times 8 \times 4^2 \equiv 384$. This anomaly results from additional $\mathbb{Z}_3$ symmetry in the group $G_{4\times 4}$. Now the translation subgroup $\mathbf{T}^2 = \mathbb{Z}_4 \times \mathbb{Z}_4$ is *not normal* and the structure of $G_{4\times 4}$ differs essentially from (1). The algorithm used by the computer algebra system **GAP** [4] gives the following structure:

$$G_{4\times 4} = \overbrace{((((\mathbb{Z}_2 \times \mathbf{D}_4) \rtimes \mathbb{Z}_2) \rtimes \mathbb{Z}_3) \rtimes \mathbb{Z}_2)}^{\text{normal closure of } \mathbf{T}^2} \rtimes \mathbb{Z}_2. \tag{2}$$

Functions on Lattices. To study the symmetry properties of a system on a lattice Γ we should consider action of the group $\mathrm{Aut}\,(\Gamma)$ on the space $\Sigma = Q^\Gamma$ of Q-valued functions on Γ, where $Q = \{0, \ldots, q-1\}$ is the set of values of lattice vertices. We shall call the elements of Σ *states* or (later in Sec. 3) *microstates*. The group $\mathrm{Aut}\,(\Gamma)$ acts nontransitively on the space Σ splitting this space into the disjoint orbits of different sizes

$$\Sigma = \bigcup_{i=1}^{N_{\text{orbits}}} O_i.$$

The action of $\mathrm{Aut}\,(\Gamma)$ on Σ is defined by $(g\varphi)(x) = \varphi(g^{-1}x)$, where $x \in V(\Gamma)$, $\varphi(x) \in \Sigma$, $g \in \mathrm{Aut}\,(\Gamma)$. Burnside's lemma counts the total number of orbits in the state space Σ

$$N_{\text{orbits}} = \frac{1}{|\mathrm{Aut}\,(\Gamma)|} \sum_{g \in \mathrm{Aut}\,(\Gamma)} q^{N^g_{\text{cycles}}},$$

where N^g_{cycles} is the number of cycles in the group element g.

Large symmetry group allows one to represent dynamics on the lattice in more compact form. For example, the automorphism group of (graph of) icosahedron, dodecahedron and buckyball is S_5, and the information about behavior of any dynamical system on these lattices can be compressed nearly in proportion to $|S_5| = 120$.

2. DETERMINISTIC SYSTEMS

Universal Property of Deterministic Evolution Induced by Symmetry. The splitting of the space Σ of functions on a lattice into the group orbits of different sizes imposes *universal restrictions* on behavior of a deterministic dynamical system for any law that governs evolution of the system. Namely, dynamical trajectories can obviously go only in the direction of *nondecreasing sizes of orbits*. In particular, *periodic trajectories* must lie *within the orbits of the same size*. Conceptually this restriction is an analog of the *second law of thermodynamics* — any isolated system may only lose information in its evolution.

Formation of Soliton-like Structures. After some lapse of time the dynamics of finite discrete system is governed by its symmetry group, that leads to appearance of *soliton-like* structures. Let us clarify the matter. Obviously phase portraits of the systems under consideration consist of attractors being limit cycles and/or isolated cycles (including limit and isolated fixed points). Let us consider the behavior of the system on a cycle. The system runs periodically over some sequence of equal size orbits. The same orbit may occur in the cycle repeatedly. For example, the isolated cycle of period 6 in Fig. 2 — where a typical phase portrait *modulo* automorphisms is presented — passes through the sequence of orbits numbered by our program as 0, 2, 4, 0, 2, 4, i.e., each orbit appears twice in the cycle.

Suppose a state $\varphi(x)$ of the system on a cycle belongs to ith orbit at some moment t_0: $\varphi(x) \in O_i$. At some other moment t the system appears again in the same orbit with the state $\varphi_t(x) = A_{t_0 t}(\varphi(x)) \in O_i$. Clearly, the evolution operator $A_{t_0 t}$ can be replaced by the action of some group element $g_{t_0 t} \in \mathrm{Aut}\,(\Gamma)$

$$\varphi_t(x) = A_{t_0 t}(\varphi(x)) = \varphi(g_{t_0 t}^{-1} x). \tag{3}$$

The element $g_{t_0 t}$ is determined uniquely *modulo* subgroup $\mathrm{Aut}(\Gamma; \varphi(x)) \subseteq \mathrm{Aut}\,(\Gamma)$ fixing the state $\varphi(x)$. Equation (3) means that the initial cofiguration (shape) $\varphi(x)$ is completely reproduced after some movement in the space Γ. Such soliton-like structures are typical of cellular automata. They are called *spaceships* in the cellular automata community.

As an illustration, let us consider the *glider* — one of the simplest spaceships of Conway's automaton «Life». This configuration moves along the diagonal of square lattice reproducing itself with one step diagonal shift after four steps in time. If one considers only translations as a symmetry group of the lattice, then, as it is clear from Fig. 1, φ_5 is the first configuration lying in the same orbit with φ_1, i.e., for the translation group $\mathbf{T}^2$ glider is a cycle running over *four* orbits.

Our program constructs the maximum possible automorphism group for any lattice. For an $N \times N$ square toric lattice this group is the above-mentioned $G_{N\times N}$ (we assume $N \neq 4$).

Now the glider is reproduced after two steps in time. As one can see from Fig. 1, φ_3 is obtained from φ_1, and φ_4 — from φ_2 by combinations of translations, 90° rotations and reflections. Thus, the glider in torus (and in the discrete plane) is a cycle located in two orbits of maximal automorphism group.

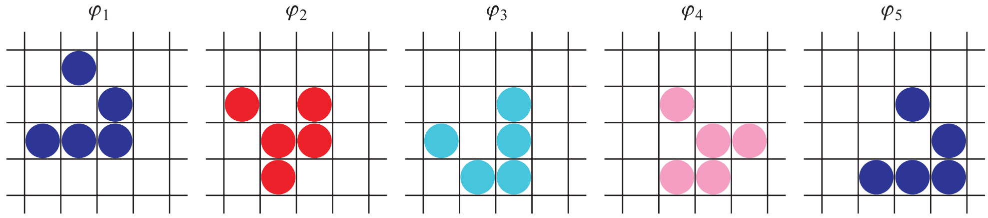

Fig. 1. Glider is a cycle in *four* group orbits over translation group $\mathbf{T}^2$, but it is a cycle in *two* orbits over maximal symmetry group $\mathbf{T}^2 \rtimes \mathbf{D}_4$

Note also that similar behavior is rather typical of continuous systems too. Many equations of mathematical physics have solutions in the form of running wave $\varphi(x - vt)$ $\left(= \varphi\left(g_t^{-1}x\right)\right.$ for Galilei group). One can also see an analogy between *spaceships* of cellular automata and *solitons* of KdV-type equations. The solitons — like shape preserving moving structures in cellular automata — often arise for rather arbitrary initial data.

Cellular Automata with Symmetric Local Rules. As an example, consider «one-time-step» cellular automata on k-valent lattices with local rules symmetric with respect to all permutations of k outer vertices of the neighborhood. This symmetry property is an immediate discrete analog of general local diffeomorphism invariance of fundamental physical theories based on continuous space. The diffeomorphism group $\mathrm{Diff}(M)$ of the *manifold* M is very special subgroup of the infinite symmetric group $\mathrm{Sym}(M)$ of the *set* M.

As we demonstrated in [5], in the binary case, i.e., if the number of vertex values $q = 2$, the automata with symmetric local rules are completely equivalent to generalized Conway's «Game of Life» automata [6] and their rules can be represented by «Birth»/«Survival» lists.

Adopting the convention that the outer points and the root point of the neighborhood are denoted $x_1, \ldots, x_k$ and x_{k+1}, respectively, we can write a *local rule* determining one-time-step evolution of the root in the form

$$x'_{k+1} = f\left(x_1, \ldots, x_k, x_{k+1}\right). \tag{4}$$

The rules obtained from each other by permutation of q elements in the set Q are equivalent since such a permutation means nothing but renaming of values. Thus, we can reduce the number of rules to consider the counted via *Burnside's lemma* number of orbits of rules (4) under the action of the group S_q. The concrete expression depends on the cyclic structure of elements of S_q. For the case $q = 2$ it is $N_{\text{rules}} = 2^{2k+1} + 2^k$.

Example of Phase Portrait. Cellular Automaton 86 on Hexahedron. The number 86 is the «little endian» representation of the bit string 01101010 containing values of x'_4 corresponding to ordered in some way symmetrized combinations of values of variables x_1, x_2, x_3, x_4. The rule can also be represented in the «Birth»/«Survival» notation as B123/S0, or as polynomial over the Galois field $\mathbb{F}_2$ (see [5]) $x'_4 = x_4 + \sigma_3 + \sigma_2 + \sigma_1$, where $\sigma_1 = x_1 + x_2 + x_3$, $\sigma_2 = x_1x_2 + x_1x_3 + x_2x_3$, $\sigma_3 = x_1x_2x_3$ are *symmetric* functions. In Fig. 2 the group orbits are represented by circles. The ordinal numbers of orbits are placed within these circles. The numbers over orbits and within cycles are sizes of the orbits. The rational number p indicates the *weight* of an element of phase portrait. In other words, p is a probability to find a system in a particular structure at random choice of state: $p =$ (*size of basin*)/(*total number of states*). Here *size of basin* is a sum of sizes of orbits involved in the structure.

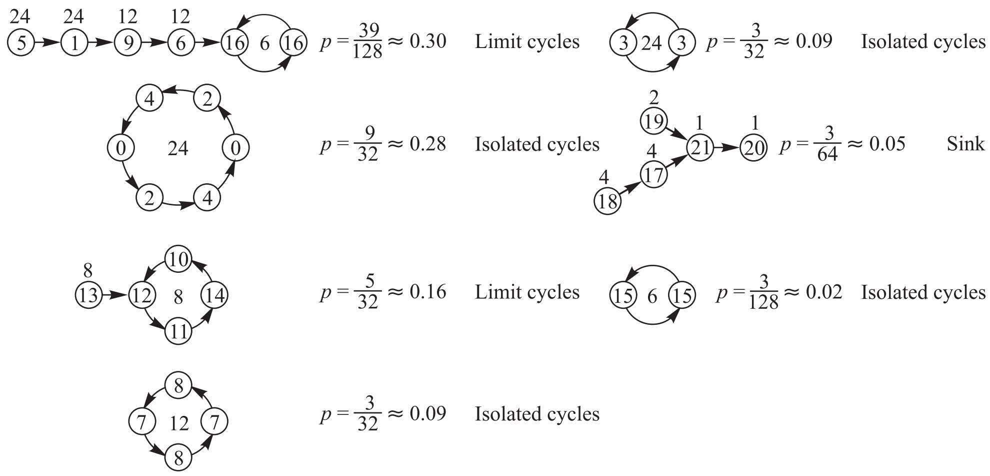

Fig. 2. Rule 86. Equivalence classes of trajectories on hexahedron

Note that most of cycles in Fig. 2 (36 out of 45 or 80%) are *spaceships*. Other computed examples also confirm that soliton-like moving structures are typical of cellular automata.

Search for Reversibility. The program is able to select automata with properties specified at input. One of such important properties is *reversibility*. In this connection we would like to mention recent works of G. 't Hooft. One of the difficulties of Quantum Gravity is a conflict between irreversibility of Gravity — information loss at the black hole — and reversibility and unitarity of the standard Quantum Mechanics. In several papers of recent years (see, e.g., [7, 8]) 't Hooft developed the approach aiming to reconcile both theories. The approach is based on the following assumptions:

- physical systems have *discrete degrees of freedom* at Planck distance scales;
- the states of these degrees of freedom form *primordial* basis of Hilbert space (with nonunitary evolution);
- primordial states form *equivalence classes*: two states are equivalent if they evolve into the same state after some lapse of time;
- the equivalence classes by construction form basis of Hilbert space with unitary evolution described by time-reversible Schrödinger equation.

In our terminology this corresponds to transition to limit cycles: in a finite time of evolution the limit cycle becomes physically indistinguishable from reversible isolated cycle — the system «forgets» its pre-cycle history. This irreversibility hardly can be found experimentally (assuming, of course, that considered models can be applied to physical reality). The system should probably spend time of order the Planck one ($\approx 10^{-44}$ s) out of a cycle and potentially infinite time on the cycle. Nowadays, the shortest experimentally fixed time is about 10^{-18} s or 10^{26} Planck units only.

Applying our program to all 136 symmetric 3-valent automata we have the following. There are two rules trivially reversible on all lattices: $85 \sim \mathrm{B0123/S} \sim x_4' = x_4 + 1$, and $170 \sim \mathrm{B/S0123} \sim x_4' = x_4$. Besides these uninteresting rules there are 6 reversible rules on *tetrahedron*: $43 \sim \mathrm{B0/S012} \sim x_4' = x_4(\sigma_2 + \sigma_1) + \sigma_3 + \sigma_2 + \sigma_1 + 1$, $51 \sim \mathrm{B02/S02} \sim x_4' = \sigma_1 + 1$, $77 \sim \mathrm{B013/S1} \sim x_4' = x_4(\sigma_2 + \sigma_1 + 1) + \sigma_3 + \sigma_2 + 1$, $178 \sim \mathrm{B2/S023} \sim$

$x_4' = x_4(\sigma_2 + \sigma_1 + 1) + \sigma_3 + \sigma_2$, $204 \sim$ B13/S13 $\sim x_4' = \sigma_1$, $212 \sim$ B123/S3 $\sim$ $x_4' = x_4(\sigma_2 + \sigma_1) + \sigma_3 + \sigma_2 + \sigma_1$. Two of the above rules, namely 51 and 204, are reversible on *hexahedron* too. There are no nontrivial reversible rules on more complicated lattices. Thus, we may suppose that 't Hooft's picture is typical of discrete dynamical systems.

3. MESOSCOPIC LATTICE MODELS

Statistical Mechanics. The state of deterministic dynamical system at any point of time is determined uniquely by previous states of the system. A Markov chain — for which transition from any state to any other state is possible with some probability — is a typical example of *nondeterministic* dynamical system. The lattice models in statistical mechanics can be regarded as special instances of Markov chains. *Stationary distributions* of these Markov chains are studied by the methods of statistical mechanics.

Mesoscopy. Nowadays much attention is paid to systems which are too large for a detailed microscopic description but too small for essential features of their behavior to be expressed in terms of classical thermodynamics. This discipline, often called *mesoscopy*, covers wide range of applications from nuclei, atomic clusters, nanotechnology to multistar systems [9, 10]. Mesoscopic systems demonstrate observable experimentally and in computation the peculiarities of behavior like heat flows from cold to hot, negative specific heat, etc. All these anomalous features have natural explanation within *microcanonical* statistical mechanics [10].

Symmetry approach to mesoscopic models is based on exact enumeration of group orbits of microstates. Since statistical studies are based essentially on different simplifying assumptions, it is important to control these assumptions by exact computation, wherever possible. Moreover, we might hope to reveal with the help of exact computation subtle details of behavior of the system under consideration.

Phase Transitions. Needs of nanotechnological science and nuclear physics attract special attention to phase transitions in finite systems. Unfortunately, classical thermodynamics and the rigorous theory of critical phenomena in homogeneous infinite systems fail at the mesoscopic level. Several approaches have been proposed to identify phase transitions in mesoscopic systems. Most accepted of them are the search of *convex intruders* [11] in the entropy versus energy diagram. In the standard thermodynamics there is a relation

$$\left.\frac{\partial^2 S}{\partial E^2}\right|_V = -\frac{1}{T^2}\frac{1}{C_V}, \tag{5}$$

where C_V is the specific heat at constant volume. It follows from (5) that $\partial^2 S/\partial E^2\big|_V < 0$ and hence the entropy versus energy diagram must be concave. Nevertheless, in mesoscopic systems there might be intervals of energy where $\partial^2 S/\partial E^2\big|_V > 0$. These intervals correspond to first-order phase transitions and are called *convex intruders*. From the point of view of standard thermodynamics one can say about phenomenon of *negative heat capacity*. A convex intruder can be found easily by computer for the discrete systems we discuss here. Let us consider three adjacent values of energy E_{i-1}, E_i, E_{i+1} and corresponding numbers of microstates $\Omega_{E_{i-1}}, \Omega_{E_i}, \Omega_{E_{i+1}}$. In our discrete case the ratio $(E_{i+1} - E_i)\,/\,(E_i - E_{i-1})$ is always rational number p/q and we can write the convexity condition for entropy in terms of numbers of microstates as easily computed inequality $\Omega_{E_i}^{p+q} < \Omega_{E_{i-1}}^{p}\Omega_{E_{i+1}}^{q}$.

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