Symmetries and Formation of Structures in Discrete Dynamical Systems

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1 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. Thus we call collections of discrete finite-valued points *discrete relations* on *abstract simplicial complexes*. Special cases of this construction are, e.g., systems of *polynomial equations* over finite fields and *cellular automata*.

In this paper we study dependence of behavior of discrete dynamical systems on graphs — one-dimensional simplicial complexes — on their symmetries. The study is based essentially on our C program for a 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.

2 Symmetries of Lattices and Functions on Lattices

Lattices. A space of discrete dynamical system will be called a *lattice*. Traditionally, the word 'lattice' is often applied to some regular system of separated points of a continuous metric space. In many problems of applied mathematics and mathematical physics both metrical relations between discrete points and existence of underlying continuous manifold do not 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* Aut (Γ) acts transitively on the set of vertices $V(\Gamma)$. Sometimes we shall depict our lattices as embedded in some continuous spaces like spheres or tori (in this case we can talk about 'dimension' of lattice). But such representations are not significant in our context and used only for vizualization.

The lattices we are concerned in this paper are shown in Fig. 1. Note that the lattices marked in Fig. 1 as "Graphene 6×4 ", "Triangular 4×6 " and "Square 5×5 " can be closed by identifications of opposite sides of rectangles in several different ways. Most natural identifications form regular graphs embeddable in the torus and in the Klein bottle. Computation shows that the Klein bottle arrangement (as well as others except for embeddable in the torus) leads to *nonhomogeneous* lattices. For example, the hexagonal lattice "Graphene 6×4 " embeddable in the Klein bottle has a 16-element symmetry group and this group splits the set of vertices into two orbits of sizes 8 and 16. Since non-transitivity of points contradicts our usual notion of space (and our definition of lattice), we shall not consider further such lattices.

It is interesting to note that the graph of hexahedron can be interpreted – as is clear from Fig. 2 – either as 4-gonal lattice in sphere or as 6-gonal lattice in torus.

Computing Automorphisms. The automorphism group of graph with n vertices may have up to n! elements. However, McKay's algorithm [3], based on efficiently arranged search tree,

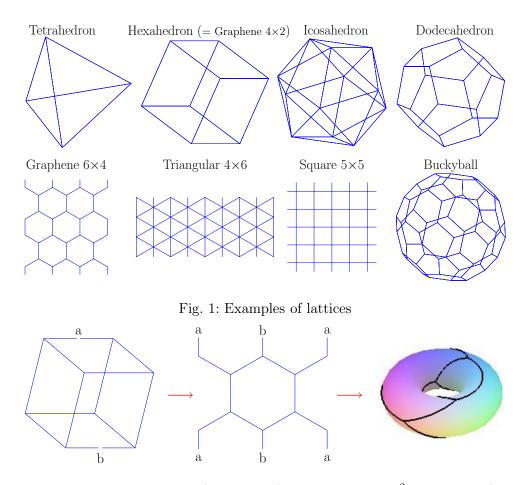


Fig. 2: The same graph forms 4-gonal (6 tetragons) lattice in sphere \mathbb{S}^2 and 6-gonal (4 hexagons) lattice in torus \mathbb{T}^2

determines the graph automorphisms by constructing small number of the group generators. This number is bounded by n-1, but usually it is much less.

In Sect. 3 we discuss the connection of formation of soliton-like structures in discrete systems with symmetries of lattices. There we consider a concrete example of the system on square lattice. 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 also assume 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

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

$$\tag{1}$$

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 are reflections. The size of $G_{N \times N}$ is

$$|G_{N\times N}| = 8N^2, \quad \text{if} \quad N \neq 4.$$

In the case N = 4 the size of the group becomes three times larger than expected

$$|G_{4\times4}| = 3\times8\times4^2 \equiv 384.$$

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 implemented in the computer algebra system GAP [4] gives the following structure

$$G_{4\times4} = \overbrace{((((\mathbb{Z}_2 \times \mathbf{D}_4) \rtimes \mathbb{Z}_2) \rtimes \mathbb{Z}_3) \rtimes \mathbb{Z}_2)}^{\text{normal closure of } \mathbf{T}^2} \rtimes \mathbb{Z}_2.$$
(2)

Functions on Lattices. To study the symmetry properties of a system on a lattice Γ , we should consider action of the group Aut (Γ) 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 Sect. 4) microstates.

The group Aut (Γ) acts non-transitively on the space Σ splitting this space into the disjoint orbits of different sizes

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

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

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

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

The large symmetry group allows one to represent dynamics on the lattice in a 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 $|S_5| = 120$.

3 Deterministic Dynamical Systems

In this section we point out a general principle of evolution of any causal dynamical system implied by its symmetry, explain formation of soliton-like structures, and consider some results of computing with symmetric 3-valent cellular automata.

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 the evolution of the system. Namely, dynamical trajectories can obviously go only in the direction of *non-decreasing 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, the phase portraits of the systems under consideration consist of attractors being limit cycles and/or isolated cycles (including limit and isolated fixed points regarded as cycles of period one). Now let us consider the behavior of the system which has come to a cycle, no matter whether the cycle is limit or isolated. 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. 4 — where a typical phase portrait *modulo* automorphisms is presented — passes through the sequence of orbits numbered¹ as 0, 2, 4, 0, 2, 4, i.e., each orbit appears twice in the cycle.

¹The program numbers orbits in the order of decreasing of their sizes and at equal sizes the lexicographic order of lexicograhically minimal orbit representatives is used.

Suppose a state $\varphi(x)$ of the system running over a cycle belongs to *i*th 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 $\varphi_t(x) = A_{t_0t}(\varphi(x)) \in O_i$. Clearly, the evolution operator A_{t_0t} can be replaced by the action of some group element $g_{t_0t} \in \text{Aut}(\Gamma)$

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

The element g_{t_0t} is determined uniquely *modulo* subgroup Aut $(\Gamma; \varphi(x)) \subseteq$ Aut (Γ) 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 for cellular automata. They are called "spaceships" in the cellular automata community.

Let us illustrate the group nature of such moving self-reproducing structures by the example of "glider" — one of the simplest spaceships of Conway's automaton "Life". This configuration moves along the diagonal of a 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. 3, 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.

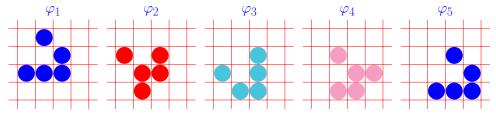


Fig. 3: Glider is cycle in *four* group orbits over translation group \mathbf{T}^2 , but it is cycle in *two* orbits over maximal symmetry group $\mathbf{T}^2 \rtimes \mathbf{D}_4$

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 $N \neq 4$, see formula (1) and subsequent discussion).

Now the glider is reproduced after two steps in time. As one can see from Fig. 3, 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 obtained from the torus as $n \to \infty$) is a cycle located in two orbits of maximal automorphism group.

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

Cellular Automata with Symmetric Local Rules. As a specific class of discrete dynamical systems, we 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 Diff(M)of the manifold M is very special subgroup of the infinite symmetric group 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, hence, their rules can be formulated in terms of "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

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

The total number of rules (4) symmetric with respect to permutations of points x_1, \ldots, x_k is equal to $q^{\binom{k+q-1}{q-1}q}$. For the case of our interest (k = 3, q = 2) this number is 256.

It should be noted that the rules obtained from each other by permutation of q elements in the set Q are equivalent since such permutation means nothing but renaming of values. Thus, we can reduce the number of rules to consider. The reduced number can be counted via *Burnside's lemma* as a 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 this gives the following number of non-equivalent rules

$$N_{rules} = 2^{2k+1} + 2^k.$$

Thus, studying a 3-valent binary case, we have to consider 136 different rules.

Example of Phase Portrait. Cellular Automaton 86. As an example, let us consider the rule 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 combinations of values of variables x_1, x_2, x_3, x_4 (assuming S₃-symmetry for x_1, x_2, x_3). 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. 4 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 (recall that all orbits included in one cycle have the same size). The rational number p indicates the weight of the corresponding element of phase portrait. In other words, p is a probability to be in an isolated cycle or to be caught by an attractor at random choice of state: p = (size of basin)/(total number of states). Here size of basin is a sum of sizes of the orbits involved in the structure.

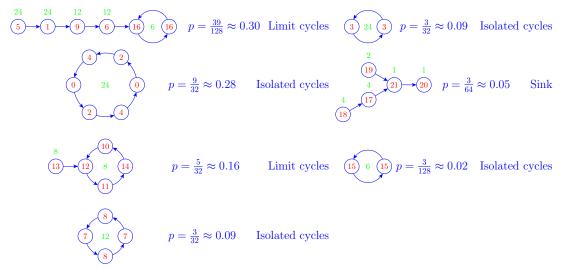


Fig. 4: Rule 86. Equivalence classes of trajectories on hexahedron. 36 of 45 cycles are "spaceships"

Note that most of cycles in Fig. 4 (36 of 45 or 80%) are "spaceships". Other computed examples also confirm that soliton-like moving structures are typical for cellular automata.

Of course, in the case of large lattices it is impractical to output full phase portraits (the program easily computes tasks with up to hundreds thousands of different structures). But it is not difficult to extract structures of interest, e.g., "spaceships" or "gardens of Eden".

Search for Reversibility. The program is able to select automata with the 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 (dissipation) at the black hole horizon - with 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 tiny (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 the evolution the limit cycle becomes physically indistinguishable from a reversible isolated cycle — the system "forgets" its pre-cycle history. Fig. 5 illustrates construction of unitary Hilbert space from primordial.

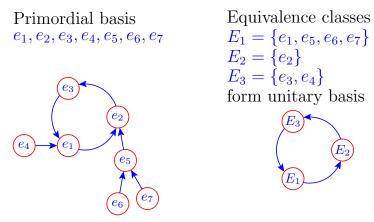


Fig. 5: Transition from primordial to unitary basis

This irreversibility can hardly 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 ($\approx 10^{-44}$ sec) out of a cycle and potentially infinite time on the cycle. Nowadays, the shortest experimentally fixed time is about 10^{-18} sec or 10^{26} Planck units only.

Applying our program to all 136 symmetric 3-valent automata, we get the following. There are two rules trivially reversible on all lattices:

- $85 \sim B0123/S \sim x'_4 = x_4 + 1,$ $170 \sim B/S0123 \sim x'_4 = x_4.$

Besides these uninteresting rules, there are 6 reversible rules on *tetrahedron*:

• 43 ~ B0/S012 ~ $x'_4 = x_4 (\sigma_2 + \sigma_1) + \sigma_3 + \sigma_2 + \sigma_1 + 1$, • 51 ~ B02/S02 ~ $x'_4 = \sigma_1 + 1$, • 77 ~ B013/S1 ~ $x'_4 = x_4 (\sigma_2 + \sigma_1 + 1) + \sigma_3 + \sigma_2 + 1$, • 178 ~ B2/S023 ~ $x'_4 = x_4 (\sigma_2 + \sigma_1 + 1) + \sigma_3 + \sigma_2$, • 204 ~ B13/S13 ~ $x'_4 = \sigma_1$, • 212 ~ B123/S3 ~ $x'_4 = x_4 (\sigma_2 + \sigma_1) + \sigma_3 + \sigma_2 + \sigma_1$.

Two of the above rules, namely 51 and 204, are reversible on *hexahedron* too. There are no nontrivial reversible rules on all other lattices from Fig. 1. Thus we may suppose that 't Hooft's picture is typical for discrete dynamical systems.

4 Lattice Models and Mesoscopic Systems

Statistical Mechanics. The state of the 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 a *non-deterministic* dynamical system. In this section we apply a symmetry approach to the lattice models in statistical mechanics. These models can be regarded as special instances of Markov chains. *Stationary distributions* of these Markov chains are studied by the methods of statistical mechanics.

The main tool of conventional statistical mechanics is the Gibbs canonical ensemble – imaginary collection of identical systems placed in a huge thermostat with temperature T. The statistical properties of canonical ensemble are encoded in the canonical partition function

$$Z = \sum_{\sigma \in \Sigma} e^{-E_{\sigma}/k_B T} \quad . \tag{5}$$

Here Σ is a set of microstates, E_{σ} is energy of microstate σ , k_B is Boltzmann's constant. The canonical ensemble is an essentially asymptotic concept: its formulation is based on approximation called "thermodynamic limit". For this reason, the canonical ensemble approach is applicable only to large (strictly speaking, infinite) homogeneous systems.

Mesoscopy. Nowadays much attention is paid to study 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 a wide range of applications from nuclei, atomic clusters, nanotechnological structures to multi-star systems [9, 10]. To study *mesoscopic* systems, one should use a more fundamental *microcanonical ensemble* instead of a canonical one. A microcanonical ensemble is a collection of identical isolated systems at fixed energy. Its definition does not include any approximating assumptions. In fact, the only key assumption of a microcanonical ensemble is that all its microstates are equally probable. This leads to the *entropy* formula

$$S_E = k_B \ln \Omega_E \quad , \tag{6}$$

or, equivalently, to the microcanonical partition function

$$\Omega_E = \mathrm{e}^{S_E/k_B} \ . \tag{7}$$

Here Ω_E is the number of microstates at fixed energy E. In what follows we will omit Boltzmann's constant assuming $k_B = 1$. Note that in the thermodynamic limit the microcanonical and canonical descriptions are equivalent and the link between them is provided by the Laplace transform. On the other hand, the mesoscopic systems demonstrate observable experimentally and in computation peculiarities of behavior like heat flows from cold to hot, negative specific heat or "convex intruders" in the entropy versus energy diagram, etc. These anomalous – from the viewpoint of canonical thermostatistics – features have a natural explanation within micro-canonical statistical mechanics [10].

Lattice Models. In this section we apply a symmetry analysis to study mesoscopic lattice models. Our approach 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.

As an example, let us consider the Ising model. The model consists of *spins* placed on a lattice. The set of vertex values is $Q = \{-1, 1\}$ and the interaction Hamiltonian is given by

$$H = -J\sum_{(i,j)} s_i s_j - B\sum_i s_i \quad , \tag{8}$$

where $s_i, s_j \in Q$; J is a coupling constant (J > 0 and J < 0 correspond to ferromagnetic and antiferromagnetic cases, respectively; the first sum runs over all edges <math>(i, j) of the lattice; B is an external "magnetic" field. The second sum $M = \sum_i s_i$ is called the magnetization. To avoid unnecessary technical details, we will consider only the case J > 0 (assuming J = 1) and B = 0 in what follows.

Since Hamiltonian and magnetization are constants on the group orbits, we can count numbers of microstates corresponding to particular values of these functions – and hence compute all needed statistical characteristics – simply by summation of sizes of appropriate orbits.

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 fails at the mesoscopic level. Several approaches have been proposed to identify phase transitions in mesoscopic systems. The most accepted one is search of "convex intruders" [11] in the entropy versus energy diagram. In the standard thermodynamics there is a relation

$$\left. \frac{\partial^2 S}{\partial E^2} \right|_V = -\frac{1}{T^2} \frac{1}{C_V} \quad , \tag{9}$$

where C_V is the specific heat at a constant volume. It follows from (9) that $\partial^2 S/\partial E^2|_V < 0$ and hence the entropy versus energy diagram must be concave. Nevertheless, in mesoscopic systems there might be intervals of energy where $\partial^2 S/\partial E^2|_V > 0$. These intervals correspond to firstorder phase transitions and are called "convex intruders". From the point of view of standard thermodynamics one can say about the phenomenon of negative heat capacity.

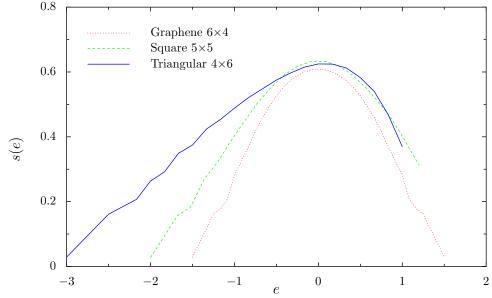


Fig. 6: Specific microcanonical entropy $s(e) = \ln(\Omega_E) / |V(\Gamma)|$ vs. energy per vertex $e = E/|V(\Gamma)|$ for the Ising model on 3-valent (*dot* line, 24 vertices), 4-valent (*dash* line, 25 vertices) and 6-valent (*solid* line, 24 vertices) tori

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

$$\Omega_{E_i}^{p+q} < \Omega_{E_{i-1}}^p \Omega_{E_{i+1}}^q$$

$$\tag{10}$$

In Fig. 6 we show the entropy-energy diagrams for lattices of different valences, namely, for 3-, 4- and 6-valent tori. In Fig. 1 these lattices are marked as "Graphene 6×4 ", "Square 5×5 " and "Triangular 4×6 ", respectively. The diagram for 3-valent torus is symmetric with respect to a change sign of energy and contains two pairs of adjacent convex intruders. One pair lies in the *e*-interval [-1.25, -0.75] and another pair lies symmetrically in [0.75, 1.25]. The 4-valent torus diagram contains two intersecting convex intruders in the intervals [-1.68, -1.36] and [-1.36, -1.04]. The 6-valent torus diagram contains a whole cascade of 5 intersecting or adjacent intruders. Their common interval is [-2.5, -0.5].

5 Summary

- A C program for the symmetry analysis of finite discrete dynamical systems has been created.
- We pointed out that trajectories of any deterministic dynamical system always go in the direction of nondecreasing sizes of group orbits. Cyclic trajectories run within orbits of the same size.
- After finite time evolution operators of the dynamical system can be reduced to group actions. This lead to formation of moving soliton-like structures "*spaceships*" in the case of cellular automata. Computer experiments show that "*spaceships*" are typical for cellular automata.
- Computational results for cellular automata with symmetric local rules allow one to suppose that reversibility is a rare property for discrete dynamical systems, and reversible systems are trivial.
- We demonstrated capability of exact computing based on symmetries in search of phase transitions for mesoscopic models in statistical mechanics.

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