Chapter 7

STRUCTURAL AND SYMMETRY ANALYSIS OF DISCRETE DYNAMICAL SYSTEMS

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Abstract

To study discrete dynamical systems of different types — deterministic, statistical and quantum — we develop various approaches. We introduce the concept of a system of discrete relations on an abstract simplicial complex and develop algorithms for analysis of compatibility and construction of canonical decompositions of such systems. To illustrate these techniques we describe their application to some cellular automata. Much attention is paid to study symmetries of the systems. In the case of deterministic systems, we reveal some important relations between symmetries and dynamics. We demonstrate that moving soliton-like structures arise inevitably in deterministic dynamical system whose symmetry group splits the set of states into a finite number of group orbits. We develop algorithms and programs exploiting discrete symmetries to study microcanonical ensembles and search phase transitions in mesoscopic lattice models. We propose an approach to quantization of discrete systems based on introduction of gauge connection with values in unitary representations of finite groups — the elements of the connection are interpreted as amplitudes of quantum transitions. We discuss properties of a quantum description of finite systems. In particular, we demonstrate that a finite quantum system can be embedded into a larger classical system. Computer algebra and computational group theory methods were useful tools in our study.

Keywords: discrete relations, cellular automata, symmetries of discrete systems, discrete gauge principle, quantization, computer algebra

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1. Introduction

There are many reasons — physical, mathematical, and conceptual — to study discrete structures. Discrete systems are important in applications — *nanostructures*, for example, by their nature are discrete, not continuous, formations. From a fundamental point of view, there are many philosophical and physical arguments that discreteness better describes physics \(^1\) at small distances than continuity which arises only as approximation or as a logical limit in considering large collections of discrete structures. As a recent development, let us mention much-discussed E. Verlinde’s thermodynamic (entropic) derivation \(^1\) of gravity and Newton’s law of inertia from G. ’t Hooft’s *holographic principle* \(^2\). The holographic principle conjectures that it is possible to describe physical events in a three-dimensional volume fully by a theory on its temporally varying two-dimensional boundary — *holographic screen* — containing finite number of discrete degrees of freedom. Entropy of these degrees of freedom, i.e., number of bits \(N\), is proportional to the area \(A\) of the screen: \(N = \frac{A c^3}{G \hbar}\). In more speculative sense, the whole universe is a finite two-dimensional information structure on the *cosmological horizon*, and observable three dimensions are only an effective description at macroscopic scales and at low energies. Verlinde shows that the laws of Newton and the Einstein equations come out directly and unavoidably from the holographic principle. The gravity appears to be an *entropic force* arising in systems with many degrees of freedom by the statistical tendency to increase its entropy — like osmosis or elasticity of polymers. Verlinde derived his results combining holography \(N = \frac{A c^3}{G \hbar}\), the equipartition rule (assumption on even distribution of energy over \(N\) bits), 1st law of thermodynamics \((dE = T dS - F dx)\) and several additional standard relations. To introduce thermodynamics, i.e., to construct *canonical partition function*, there is no need to know details of microscopic dynamics. It suffices to know about energy and number of states. Of course, the fundamental problem about laws governing bit dynamics on holographic screens remains unsolved. Since Planck scales are experimentally unavailable — the Planck length is about \(10^{-35}\) meters, i.e., far below the spacial resolution of particle accelerators (nowadays about \(10^{-18}\) meters) — the construction and study of various discrete dynamical models is one of the possible approaches.

In this chapter we consider three types of discrete dynamical systems: deterministic, mesoscopic statistical and quantum.

We begin with a general discussion of dyscrete dynamical systems. The most fundamental concepts are a discrete time and a set of states evolving in the time. A space is considered as a derived concept providing the set of states with the specific structure of a set of functions on the points of space with values in some set of local states. We give an illustration of how a space-time may arise in simple models of discrete dynamics. Then we discuss symmetries of space and local states and how these symmetries can be combined into a single group of symmetries of the system as a whole.

We introduce the concept of a system of *discrete relations on an abstract simplicial*
and explain how any system of discrete relations — subsets of Cartesian products of finite sets — acquires the structure of an abstract simplicial complex. This general concept covers many discrete mathematical structures. In particular, it can be considered as generalization of cellular automata or as a set-theoretical analog of systems of polynomial equations — if all factors of the Cartesian product are sets with the same number of elements and this number is \textit{prime power}, than any relation can be expressed by polynomial equation. We describe algorithms for analysing \textit{compatibility} and constructing \textit{canonical decompositions} of discrete relations. As an illustration, we give results of application of the algorithms to some cellular automata, namely, Conway’s automaton \textit{Game of Life} and Wolfram’s \textit{elementary cellular automata}. For many of the latter automata the canonical decomposition allows to obtain either general solutions in closed form or important information on their global behavior.

Symmetry is a property of fundamental importance for any mathematical or physical structure. Many real world discrete systems, e.g., carbon nanostructures like graphenes and fullerenes, are highly symmetric formations. Symmetries play essential role in the dynamics of the systems. In this chapter we consider connection between symmetries of discrete dynamical systems on graphs — 1-dimensional simplicial complexes — and their dynamics \cite{5,6}. In the case of \textit{deterministic dynamical systems}, such as cellular automata, non-trivial connections between the lattice symmetries and dynamics are revealed. In particular, we show that formation of moving soliton-like structures — typical examples are “spaceships” in cellular automata — is a direct result of the existence of non-trivial symmetry.

We developed also algorithms exploiting symmetries for computing microcanonical partition functions and for searching phase transitions in \textit{mesoscopic lattice models}.

We consider a class of discrete dynamical models allowing quantum description \cite{7}. Our approach to quantization consists in introduction of gauge connection with values in unitary representation (not necessarily 1-dimensional) of some group of \textit{internal symmetries} — the elements of the connection are interpreted as amplitudes of quantum transitions. The standard quantization is a special case of this construction — Feynman’s path amplitude $e^{i \int L dt}$ can be interpreted as parallel transport with values in (1-dimensional) fundamental representation $U(1)$ of the group of phase transformations. For discrete systems it is natural to take a \textit{finite} group as the \textit{quantizing} group, in this case all manipulations — in contrast to the standard quantization — remain within the framework of constructive discrete mathematics requiring no more than the ring of \textit{algebraic integers} (and sometimes the quotient field of this ring). On the other hand, the standard quantization can be approximated by taking 1-dimensional representations of large enough finite groups.

Any approach to quantization leads ultimately to unitary operators acting on a Hilbert space. We discuss peculiarities of quantum description of finite systems, under the assumption that the operators describing quantum behavior are elements of unitary representations of finite groups. We show that in this case any quantum problem can be embedded into a classical one with a larger space of representation.

Computer algebra and computational group theory \cite{8} methods turned out to be quite useful tools in our study of discrete systems.
2. Discrete Dynamics

Generally, a discrete dynamical system is a set \( S = \{s_1, \ldots, s_N\} \) of distinguishable states evolving in discrete time \( t \in \mathbb{T} \cong \mathbb{Z} = \{\ldots, -1, 0, 1, \ldots\} \), i.e., evolution or history is an element of the set \( \mathcal{E} = S^\mathbb{T} \). Dynamics is determined by some evolution rule connecting the current state \( s_t \in S \) of the system with its prehistory \( s_{t-1}, s_{t-2}, s_{t-3}, \ldots \). Different types of evolution rules are possible. We shall consider here the following types of discrete dynamics.

- **Evolution rule of deterministic dynamical system** is a functional relation. This means that the current state is a function of the prehistory:

  \[
  s_t = F(s_{t-1}, s_{t-2}, s_{t-3}, \ldots).
  \]  

  Cellular automaton is a typical example of deterministic dynamical system.

- **Statistical lattice model** is a sort of non-deterministic dynamical system. This is a special case of Markov chain. In statistical lattice model transition from one state to any other is possible with probability controlled by a Hamiltonian.

- **Quantum system** is another important type of non-deterministic dynamical system. The probabilities of transitions between states are expressed in terms of complex-valued transition amplitudes.

Symmetries play an important — central in the case of quantum systems — role in dynamical systems. So we assume the existence of a non-trivial group \( W = \{w_1 = 1, w_2, \ldots, w_{N_W}\} \) acting on the set of states \( S : W \leq \text{Sym}(S) \). Action of the group \( W \) splits the set of states \( S \) into orbits of different sizes: \( S = \bigsqcup_i O_i \) (disjoint union).

2.1. Discrete Dynamical Models with Space

In applications the set of states \( S \) usually has a special structure of a set of functions on some space. The following constructions form the basis for all types of dynamical systems we consider in this chapter:

1. **Space** is a discrete (basically finite) set of points \( X = \{x_1, x_2, \ldots, x_{N_X}\} \) provided with the structure of an abstract regular \((k\text{-valent})\) graph.

2. **Space symmetry group** \( G = \{g_1 = 1, g_2, \ldots, g_{N_G}\} \) is the graph automorphism group: \( G = \text{Aut}(X) \leq \text{Sym}(X) \). We assume that \( G \) acts transitively on \( X \).

3. **Local space symmetry group** is defined as the stabilizer of a vertex \( x_i \) in the space group \( G \): \( g \in G_{\text{loc}} = \text{Stab}_G(x) \) means \( x_i g = x_i \). Due to the transitivity all such subgroups are isomorphic and we shall denote the isomorphism class by \( G_{\text{loc}} \). This is subgroup of the space symmetry group: \( G_{\text{loc}} \leq G \).

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[1] We denote the identity elements by 1 for all groups throughout this chapter.

[2] We write group actions on the right. This, more intuitive, convention is adopted in both GAP and Magma – the most widespread computer algebra systems with advanced facilities for computational group theory.
4. Points \( x \in X \) take values in a finite set \( \Sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_{N_\Sigma}\} \) of local states.

5. Internal symmetry group \( \Gamma = \{\gamma_1 = 1, \gamma_2, \ldots, \gamma_{N_\Gamma}\} \) is a group \( \Gamma \leq \text{Sym} (\Sigma) \) acting on the set of local states \( \Sigma \).

6. States of the whole system are functions \( \sigma(x) \in \Sigma^X = \mathcal{S} \), and the set of evolutions takes the form \( \mathcal{E} = (\Sigma^X)^T = \Sigma^{X \times T} \).

7. We define the whole symmetry groups \( W \) unifying space \( G \) and internal \( \Gamma \) symmetries as equivalence classes of split group extensions of the form

\[ 1 \rightarrow \Gamma^X \rightarrow W \rightarrow G \rightarrow 1, \]

where \( \Gamma^X \) is the set of \( \Gamma \)-valued functions on \( X \). (More detailed description of this construction see in Sect. 2.1.3.)

The separation of the set \( \mathcal{S} \) into “space” and “local states” is not fundamental — it is model- and interpretation-dependent. An example of a system with a somewhat non-standard notion of space is a quantum computer. Here the space \( X \) is the set of \( N_X \) qubits, the set of local states \( \Sigma \) is \( \{0, 1\} \). The whole set of states \( \mathcal{S} = \{0, 1\}^X \) contains \( 2^{N_X} \) elements.

### 2.1.1. Example of Discrete Model with Emergent Space-time.

Modern fundamental theories, in particular the string theory, provide evidence that space is an emergent phenomenon \( \mathbb{[9]} \), arising from more basic concepts. We demonstrate here that if we have a concept of time then discrete space-time structures may arise under very simple and general assumptions. It is sufficient to have a time-labelled sequence of events and ability to distinguish different types of the events. Then space dimensions arise as the counters of events of different types.

Let us consider a set of states (symbols) \( \Sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_{N+1}\} \) and assume that it is possible to observe the sequences (histories) \( h = s_0, s_1 \ldots s_t \), where \( s_i \in \Sigma \). Let us define a space-time point \( p \) as equivalence class of sequences with equal numbers of occurrences of each symbol, i.e., \( p \) is a “commutative monomial” of the total degree \( t \) described by \( N+1 \) non-negative integers: \( p = (n_1, \ldots, n_{N+1}), \ n_1 + \cdots + n_{N+1} = t, \ n_i \in \mathbb{Z}_{\geq 0} \) is multiplicity of symbol \( \sigma_i \) in the history \( h \). The concepts of “causality” and “light cones” arises naturally. The “speed of light limitation” is simply impossibility to get more than \( t \) symbols (“perceptions”) in \( t \) observations — in terms of monomials the “past light cone” is the set of divisors of the monomial \( p \), the “future light cone” is the set of its multiples, see Fig. 1.

The union of all possible histories form a causal network. As to modelling continuous Euclidean spaces by this structure, the system of discrete points can be embedded into a continuum in many different ways: as a set of discrete points into a continuous space of arbitrary non-zero dimension \( \mathbb{[4]} \), as a network into a three-dimensional space \( \mathbb{[6]} \).

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\( ^5 \)For example, the map \( p \rightarrow \alpha_1 n_1 + \cdots + \alpha_{N+1} n_{N+1} \in \mathbb{R}^3 \), where \( \alpha_i \) are independent irrationals, provides one-to-one embedding of the set of points into \( \mathbb{R}^3 \).

\( ^6 \)A network, as a locally finite 1-dimensional simplicial complex, can always be embedded into \( \mathbb{R}^3 \).
Space-time point $p$ is equivalence class of paths with equal numbers of $n_1, n_2, \ldots, n_{N+1}$.

The identification can be any causality-respecting projection onto the set $t = \text{const}$. To construct an illustrative discrete model of this section we use the following projection. Let us identify the symbols $\sigma_i$ with $N + 1$ unit vectors forming regular simplex in an $N$-dimensional Euclidean space. These systems of vectors (network generating sets) look like $\sigma_1, \sigma_2, \sigma_3$ for $N = 1, 2, 3$, respectively. The space lattices generated by these sets in four time steps ($t = 4$) for the cases $N = 2$ and $N = 3$ are shown in the figure.

With these prerequisites, let us construct a simple physical model in 1-dimensional space ($N = 1$). We have $\Sigma = \{\sigma_1, \sigma_2\} = \{\rightarrow, \leftarrow\}$, $t = n_1 + n_2 \in \mathbb{Z}_{\geq 0}$. Let us add a little physics by imposing the structure of Bernoulli trials on the sequences $h = s_0 s_1 \cdots s_t$. Namely, let us introduce probabilities $p_1$ and $p_2$ ($p_2 + p_1 = 1$) for possible outcomes $\sigma_1$ and $\sigma_2$ of a single trial. The probability of a separate history $h$ is described by the binomial distribution

$$P(n_1, n_2) = \frac{(n_1 + n_2)!}{n_1!n_2!} p_1^{n_1} p_2^{n_2}. \quad (2)$$

From this model we can see that the behavior of a discrete system may differ essentially.
from the behavior of its continuous approximation. Applying Stirling’s approximation to (2) and introducing new variables $x = n_1 - n_2$, $v = p_1 - p_2$ — let us call them “space” and “velocity”, respectively — we obtain

$$P(x, t) \approx \tilde{P}(x, t) = \frac{1}{\sqrt{1 - v^2}} \sqrt{\frac{2}{\pi t}} \exp \left\{ -\frac{1}{2t} \left( \frac{x - vt}{\sqrt{1 - v^2}} \right)^2 \right\}. \quad (3)$$

This is the fundamental solution of the heat (also known as diffusion or Fokker–Planck\footnote{The name of the equation depends on interpretation of the function $\tilde{P}(x, t)$.} equation:

$$\frac{\partial \tilde{P}(x, t)}{\partial t} + v \frac{\partial \tilde{P}(x, t)}{\partial x} = \frac{(1 - v^2)}{2} \frac{\partial^2 \tilde{P}(x, t)}{\partial x^2}. \quad (4)$$

Note that expression (3) — due to the velocity limits $-1 \leq v \leq 1$ in our model — contains “relativistic” fragment $\frac{x - vt}{\sqrt{1 - v^2}}$. Note also that at $|v| = 1$ equation (4) is reduced to the wave equation

$$\frac{\partial \tilde{P}(x, t)}{\partial t} \pm \frac{\partial \tilde{P}(x, t)}{\partial x} = 0. \quad (5)$$

Now let us set a problem as is typical in mechanics: find extremal trajectories connecting two fixed points $(0, 0)$ and $(X, T)$. As a version of the “least action principle”, we adopt here the search of trajectories of maximum probability. The probability of trajectory connecting the points $(0, 0)$ and $(X, T)$ and passing through some intermediate point $(x, t)$ is the following conditional probability

$$P_{(0,0) \to (x,t) \to (X,T)} = \frac{P(x, t)P(X - x, T - t)}{P(X, T)} = \frac{t!(T - t)!(\frac{T - X}{2})!(\frac{T + X}{2})!}{(\frac{t - x}{2})!(\frac{t + x}{2})!(\frac{T - t - X}{2})!(\frac{T - t + X}{2})!T!}. \quad (6)$$

The conditional probability computed for approximation (3) takes the form

$$\tilde{P}_{(0,0) \to (x,t) \to (X,T)} = \frac{T}{\sqrt{\frac{2}{\pi}(1 - v^2)tT(T - t)}} \exp \left\{ -\frac{(Xt - xt)^2}{2(1 - v^2)tT(T - t)} \right\}. \quad (7)$$

One can see essential differences between (6) and (7):

- exact probabilities (6) do not depend on the velocity $v$ (or, equivalently, on the probabilities $p_1$, $p_2$ of a single trial), whereas (7) contains artificial dependence,

- it is easy to check that expression (6) allows many trajectories with the same maximum probability, whereas extremals of (7) are deterministic trajectories, namely, straight lines $x = \frac{X}{T} t$. This is a typical example of emergence of deterministic behaviour as a result of the law of large numbers approximation.
2.1.2. Space Symmetries in More Detail.

A space $X$ in our models has the structure of a graph. Graphs — we shall call them also lattices — are sufficient for all our purposes. In particular, they are adequate to introduce gauge and quantum structures. The symmetry group of the space $X$ is the graph automorphism group $G = \text{Aut}(X)$. The automorphism group of a graph with $n$ vertices may have up to $n!$ elements. Nevertheless, the most efficient currently algorithm designed by B. McKay \cite{10} determines the graph automorphisms by constructing compact set (no more than $n - 1$ elements, but usually much less) of generators of the group.

Very often dynamics of a model is expressed in terms of rules defined on the neighborhoods of lattice vertices. For this sort of models with locally defined evolution rules — typical examples are cellular automata and the Ising model — the above mentioned group of local symmetries $G_{\text{loc}}$ is essential. Local rules are defined on orbits of $G_{\text{loc}}$ on edges from the neighborhoods of points $x$. Fig. 2 shows the symmetry groups $G$ and $G_{\text{loc}} \leq G$ for some carbon and hydrocarbon molecules.

\begin{align*}
\text{Tetrahedrane } & C_4H_4 \\
G & = \text{Sym}(4) \\
G_{\text{loc}} & = D_6 \cong \text{Sym}(3)
\end{align*}

\begin{align*}
\text{Cubane } & C_8H_8 \\
G & = \mathbb{Z}_2 \times \text{Sym}(4) \\
G_{\text{loc}} & = D_6
\end{align*}

\begin{align*}
\text{Dodecahedrane } & C_{20}H_{20} \\
G & = \mathbb{Z}_2 \times \text{Alt}(5) \\
G_{\text{loc}} & = D_6
\end{align*}

\begin{align*}
\text{Fullerene } & C_{60} \\
G & = \mathbb{Z}_2 \times \text{Alt}(5) \\
G_{\text{loc}} & = \mathbb{Z}_2
\end{align*}

\begin{align*}
\text{Toric graphene } n \times m \\
G & = D_6 \times D_{2m} \\
G_{\text{loc}} & = \mathbb{Z}_2 \\
[n \to \infty] & G_{\text{loc}} = D_6
\end{align*}

Figure 2. Symmetries of 3-valent (hydro)carbon nanostructures.

Let us consider the role of the local group $G_{\text{loc}}$ in more detail using the buckyball as an example. The incarnations of this 3-valent graph include in particular:

\begin{itemize}
  \item the Caley graph of the icosahedral group $\text{Alt}(5)$ (in mathematics);
  \item the molecule of fullerene $C_{60}$ (in carbon chemistry).
\end{itemize}

\footnotetext{The classical book by F. Klein \cite{11} is devoted entirely to this group.}
The symmetry group of the buckyball is \( G = \text{Aut} (X) = \mathbb{Z}_2 \times \text{Alt}(5) \). The neighborhood of a vertex \( x_i \) takes the form

![Diagram of a vertex with neighborhood edges]

The stabilizer of \( x_i \) is \( G_{\text{loc}} = \text{Stab}_G (x_i) = \mathbb{Z}_2 \).

The set of neighborhood edges contains three elements:

\[
E_i = \{ e_{1,i} = (x_i, x_{1,i}), e_{2,i} = (x_i, x_{2,i}), e_{3,i} = (x_i, x_{3,i}) \}.
\]

The set of orbits of \( G_{\text{loc}} \) on \( E_i \) consists of two orbits:

\[
\Omega_i = \{ \omega_{1,i} = \{ e_{1,i}, e_{2,i} \}, \omega_{2,i} = \{ e_{3,i} \} \},
\]

i.e., the stabilizer does not move the edge \((x_i, x_{3,i})\) and swaps \((x_i, x_{1,i})\) and \((x_i, x_{2,i})\).

This asymmetry results from different roles the edges play in the structure of the buckyball: \((x_i, x_{1,i})\) and \((x_i, x_{2,i})\) are edges of a pentagon adjacent to \( x_i \), whereas \((x_i, x_{3,i})\) separates two hexagons; in the carbon molecule \( C_{60} \) the edge \((x_i, x_{3,i})\) corresponds to the double bond, whereas others are the single bonds.

Naturally formulated local rules determining behavior of a system must respect decompositions of neighborhoods into the orbits of the group of local symmetries. For example, the Hamiltonian of the Ising model on the buckyball must depend on two, generally different, coupling constants \( J_{12} \) and \( J_3 \). Moreover, the coupling constants may be of different types — ferromagnetic or antiferromagnetic — and this may lead to interesting behavior of the model. Such natural Hamiltonian should take the form

\[
H_{\text{bucky}} = -\frac{1}{2} \sum_i s_i [J_{12} (s_{1,i} + s_{2,i}) + J_3 s_{3,i}] - B \sum_i s_i,
\]

where \( s_i, s_{1,i}, s_{2,i}, s_{3,i} \in \Sigma = \{-1, 1\} \). In a similar way the local rule for a cellular automaton on the buckyball must have the form

\[
x'_i = f (x_i, x_{1,i}, x_{2,i}, x_{3,i}),
\]

where function \( f \) must be symmetric with respect to variables \( x_{1,i} \) and \( x_{2,i} \), i.e.,

\[
f (x_i, x_{1,i}, x_{2,i}, x_{3,i}) \equiv f (x_i, x_{2,i}, x_{1,i}, x_{3,i}).
\]

### 2.1.3. Unification of Space and Internal Symmetries.

Having the groups \( G \) and \( \Gamma \) acting on \( X \) and \( \Sigma \), respectively, we can combine them into a single group \( W \leq \text{Sym} (\Sigma^X) \) which acts on the states \( \mathcal{S} = \Sigma^X \) of the whole system. The group \( W \) can be identified, as a set, with the Cartesian product \( \Gamma^X \otimes G \), where \( \Gamma^X \) is the set of \( \Gamma \)-valued functions on \( X \). That is, every element \( u \in W \) can be represented in the form \( u = (\alpha (x), a) \), where \( \alpha (x) \in \Gamma^X \) and \( a \in G \). A priori there are different possible ways to combine \( G \) and \( \Gamma \) into a single group. So selection of possible combinations should be guided by some natural (physical) reasons. General arguments convince that the required combination \( W \) should be a split extension of the group \( G \) by the group \( \Gamma^X \). In physics, it
is usually assumed that the space and internal symmetries are independent, i.e., W is the direct product $\Gamma^X \times G$ with action on $\Sigma^X$ and multiplication rules:

$$\sigma(x)(\alpha(x), a) = \sigma(x)\alpha(x) \quad \text{action},$$

$$\sigma(x)(\alpha(x), a) = \sigma(xa^{-1})\alpha(xa^{-1}),$$

$$\alpha(x), a)(\beta(x), b) = (\alpha(x)\beta(x), ab) \quad \text{multiplication}. \quad (9)$$

Another standard construction is the wreath product $\Gamma \wr X \rtimes G$ having a structure of the semidirect product $\Gamma \rtimes X \rtimes G$ with action and multiplication

$$\sigma(x)(\alpha(x), a) = \sigma(xa)\alpha(xa^{-1}),$$

$$\alpha(x), a)(\beta(x), b) = (\alpha(x)\beta(xa), ab). \quad (10)$$

These examples are generalized by the following

**Statement.** There are equivalence classes of split group extensions

$$1 \to \Gamma^X \to W \to G \to 1 \quad (11)$$

determined by antihomomorphism $\mu : G \to G$. The equivalence is described by arbitrary function $\kappa : G \to G$. The explicit formulas for main group operations — action on $\Sigma^X$, multiplication and inversion — are

$$\sigma(x)(\alpha(x), a) = \sigma(x\mu(a))\alpha(x\kappa(a)), \quad \alpha(x), a)(\beta(x), b) = \left(\alpha(x\kappa(ab^{-1})\mu(b)\kappa(a))\beta(x\kappa(ab^{-1}\kappa(b)), ab\right), \quad (12)$$

$$\left(\alpha(x), a\right)^{-1} = \left(\alpha\left(x\kappa(a^{-1})\mu(a^{-1}\kappa(a))^{-1}, a^{-1}\right)\right). \quad (13)$$

This statement follows from the general description of the structure of split extensions of a group $G$ by a group $H$: all such extensions are determined by the homomorphisms from $G$ to $\text{Aut}(H)$ (see, e.g., [12]). Specializing this description to the case when $H$ is the set of $\Gamma$-valued function on $X$ and $G$ acts on arguments of these functions we obtain our statement. The equivalence of extensions with the same antihomomorphism $\mu$ but with different functions $\kappa$ is expressed by the commutative diagram

$$
\begin{array}{ccccccc}
1 & \longrightarrow & \Gamma^X & \longrightarrow & W & \longrightarrow & G & \longrightarrow & 1 \\
\downarrow & & \downarrow & & \downarrow & & \downarrow & & \\
1 & \longrightarrow & \Gamma^X & \longrightarrow & W' & \longrightarrow & G & \longrightarrow & 1
\end{array}, \quad (15)

where the mapping $K$ takes the form $K : (\alpha(x), a) \mapsto (\alpha(x\kappa(a)), a)$.

Note that the standard direct and wreath products are obtained from this general construction by choosing antihomomorphisms $\mu(a) = 1$ and $\mu(a) = a^{-1}$, respectively. As to the arbitrary function $\kappa$, the choices $\kappa(a) = 1$ and $\kappa(a) = a^{-1}$, respectively, are generally used in the literature.

\footnote{The term ‘antihomomorphism’ means that $\mu(a)\mu(b) = \mu(ba)$.}
In our computer programs (written in C) the group \( W \) is specified by two groups \( G \) and \( \Gamma \) and two functions \( \mu(a) \) and \( \kappa(a) \) implemented as arrays. It is convenient in computations to use the following specialization: \( \mu(a) = a^{-m} \) and \( \kappa(a) = a^k \). For such a choice formulas (12), (14) take the form

\[
\sigma(x) (\alpha (x), a) = \sigma (xa^{-m} \alpha x a^k), \tag{16}
\]

\[
(\alpha (x), a) (\beta (x), b) = \left( \alpha \left( x(ab)^{-k-m} a^{k+m} \right) \beta \left( x(ab)^{-k} b^k \right), ab \right), \tag{17}
\]

\[
(\alpha(x), a)^{-1} = \left( \alpha \left( xa^{2k+m} \right)^{-1}, a^{-1} \right). \tag{18}
\]

Here \( k \) is arbitrary integer, but \( m \) is restricted only to two values: \( m = 0 \) and \( m = 1 \), i.e., such specialization does not cover other than, respectively, direct and wreath types of split extentions. On the other hand, the antihomomorphisms \( \mu(a) = 1 \) and \( \mu(a) = a^{-1} \) exist for any group, while others depend on the particular structure of a group. Note that actions of \( G \) on any function \( f(x) \) are called trivial and natural for \( \mu(a) = 1 \) and \( \mu(a) = a^{-1} \), respectively.

### 3. Structural Analysis of Discrete Relations

The methods of compatibility analysis, such as the Gröbner basis computation or reduction to involutive form, are widely used to study systems of polynomial and differential equations. In this section we develop similar techniques for discrete systems, in particular, for cellular automata.

Let us consider the Cartesian product \( \Sigma^n = \Sigma_1 \times \Sigma_2 \times \cdots \times \Sigma_n \), i.e., the set of ordered \( n \)-tuples \( (\sigma_1, \sigma_2, \ldots, \sigma_n) \), with \( \sigma_i \in \Sigma_i \) for each \( i \). By definition, \( n \)-ary relation is any subset of the \( n \)-dimensional hyperparallelepiped \( \Sigma^n \). We assume that \( \Sigma_i \) are finite sets of \( q_i = |\Sigma_i| \) elements that we shall call states.

We can treat \( n \) dimensions of the hyperparallelepiped \( \Sigma^n \) as elements of a set of points \( X = \{x_1, x_2, \ldots, x_n\} \). To make this initially amorphous set into a “space” (or “space-time”) we should provide \( X \) with a structure determining how “close” to each other are different points. The relevant mathematical abstraction of such a structure is an abstract simplicial complex. The natural concept of space assumes the homogeneity of its points. This means that there exists a symmetry group acting transitively on \( X \), i.e., providing possibility to “move” any point into any other. The homogeneity is possible only if all \( \Sigma_i \) are equivalent. Let us denote the equivalence class by \( \Sigma \). We can represent \( \Sigma \) canonically in the form \( \Sigma = \{0, \ldots, q - 1\} \), \( q = |\Sigma| \).

If the number of states is a prime power, \( q = p^m \), we can additionally equip the set \( \Sigma \) with the structure of the Galois field \( \mathbb{F}_q \). Using the functional completeness of polynomials — this means that any function can be represented as polynomial — over finite fields \([13]\), we can represent any \( k \)-ary relation on \( \Sigma \) as a set of zeros of some polynomial belonging to the ring \( \mathbb{F}_q [x_1, \ldots, x_k] \). Thus, the set of relations can be regarded as a system of polynomial equations. Although this description is not necessary (and does not work, if \( \Sigma_i \) are different sets or \( q \) is not prime power), it is useful due to our habit to employ polynomials wherever
possible and capability of applying different advanced tools of polynomial algebra, such as, for example, the Gröbner bases.

An abstract simplicial complex (see, e.g., [14]) \( K = (X, \Delta) \) is determined by a set of points \( X = \{x_1, x_2, \ldots, x_n\} \) and an assembly \( \Delta \) of subsets of \( X \), which are called simplices, such that (a) for all \( x_i \in X \ \{x_i\} \in \Delta \) and (b) if \( \tau \subseteq \delta \in \Delta \), then \( \tau \in \Delta \). The subsets of a simplex — they are also simplices due to (b) — are called faces. Condition (a) means that all one-element subsets are simplices. Clearly, the structure of the complex \( K \), i.e., the set \( \Delta \), is uniquely determined by the simplices that are maximal by inclusion. Dimension of a simplex \( \delta \) is the number \( \dim \delta = |\delta| - 1 \). This definition is motivated by the fact that \( k + 1 \) points immersed in the general position into the Euclidean space \( \mathbb{R}^{n+1} \) form a \( k \)-dimensional convex polyhedron. The dimension of a complex \( K \) is defined as the maximum dimension of all simplices in \( K \): \( \dim K = \max_{\delta \in \Delta} \dim \delta \). From the point of view of abstract combinatorial topology, no matter how the complex can be immersed into the space \( \mathbb{R}^n \) — it is essential only how its simplices are connected with each other. However, it follows from the Nöbeling–Pontryagin theorem that any (locally finite) abstract \( k \)-dimensional complex can be geometrically realized in the space \( \mathbb{R}^{2k+1} \). We will show below that, for any \( n \)-ary relation \( R \subseteq \Sigma^n \), one can regularly and uniquely construct some abstract simplicial complex.

### 3.1. Basic Definitions and Constructions

In addition to \( k \)-simplices, which are singled out sets of \( k + 1 \) points, we need to consider arbitrary sets of point. For brevity, we shall call sets containing \( k \) points by \( k \)-sets. Dealing with systems of relations defined on different sets of points, it is necessary to establish correspondence between the points and dimensions of the hypercube \( \Sigma^k \). This is achieved by using exponential notation. The notation \( \Sigma^{\{x_i\}} \) fixes \( \Sigma \) as the set of values of the point \( x_i \). For the \( k \)-set \( \delta = \{x_1, \ldots, x_k\} \), we introduce the notation \( \Sigma^\delta = \Sigma^{\{x_1\}} \times \ldots \times \Sigma^{\{x_k\}} \). The set \( \delta \) is called the domain of the relation \( R^\delta \). We will call the whole hypercube \( \Sigma^\delta \) a trivial relation. Accordingly, \( R^\delta \subseteq \Sigma^\delta \) denotes a relation given on the set of points \( \delta \).

#### 3.1.1. Relations.

Thus, we have:

**Definition 1** (relation). A relation \( R^\delta \) on the set of points \( \delta = \{x_1, \ldots, x_k\} \) is any subset of the hypercube \( \Sigma^\delta \); i.e., \( R^\delta \subseteq \Sigma^\delta \). The relation \( R^\delta \) can be regarded as the Boolean-valued function \( R^\delta : \Sigma^\delta \to \{0, 1\} \). We can think of \( x_i \)'s as variables taking values in \( \Sigma \) and write the relation as

\[
a = R^\delta (x_1, \ldots, x_k), \quad a \in \{0, 1\}.
\]

An important special case of relations:

**Definition 2** (functional relation). A relation \( R^\delta \) on the set of points \( \delta = \{x_1, \ldots, x_k\} \) is called functional if there is a position \( i \in \{1, \ldots, k\} \) such that for any \( \sigma_1, \ldots, \sigma_{i-1}, \sigma_{i+1}, \ldots, \sigma_k, \zeta, \tau \in \Sigma \) from \((\sigma_1, \ldots, \sigma_{i-1}, \zeta, \sigma_{i+1}, \ldots, \sigma_k) \in R^\delta \) and \((\sigma_1, \ldots, \sigma_{i-1}, \tau, \sigma_{i+1}, \ldots, \sigma_k) \in R^\delta \)
it follows that $\varsigma = \tau$.

In terms of variables the functional relation $R^\delta$ can be written in the form

$$x_i = F(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_k), \quad \text{where} \quad F : \Sigma^\delta \{x_i\} \to \Sigma.$$  

We need to be able to extend relations from subsets of points to larger sets:

**Definition 3** (extension of relation). For given set of points $\delta$, its subset $\tau \subseteq \delta$ and relation $R^\tau$ on the subset $\tau$, we define the *extension* of $R^\tau$ as the relation

$$R^\delta = R^\tau \times \Sigma^\delta \setminus \tau.$$  

This definition, in particular, allows the relations $R^{\delta_1}, \ldots, R^{\delta_m}$ defined on different domains to be extended to the common domain, i.e., to the union $\delta_1 \cup \cdots \cup \delta_m$.

Logical implications of the relations are defined in a natural way:

**Definition 4** (consequence of relation). A relation $Q^{\delta}$ is called a *consequence* of the relation $R^{\delta}$ if $R^{\delta} \subseteq Q^{\delta} \subseteq \Sigma^{\delta}$; i.e., $Q^{\delta}$ is arbitrary superset of the set $R^{\delta}$.

The relation $R^{\delta}$ may have many different consequences: their total number (including $R^{\delta}$ itself and the trivial relation $\Sigma^{\delta}$) is evidently equal to $2^{\mid \Sigma^{\delta} \mid - \mid R^{\delta} \mid}$.

It is natural to single out the consequences that can be reduced to relations on smaller sets of points:

**Definition 5** (proper consequence). A nontrivial relation $Q^{\tau}$ is called the *proper consequence* of the relation $R^{\delta}$ if $\tau$ is a proper subset of $\delta$ (i.e., $\tau \subset \delta$) and the relation $Q^{\tau} \times \Sigma^\delta \setminus \tau$ is a consequence of $R^{\delta}$.

We call relations that have no proper consequences the *prime relations*.

### 3.1.2. Compatibility of Systems of Relations.

The compatibility of a system of relations can naturally be defined by the intersection of their extensions to the common domain:

**Definition 6** (base relation). The *base relation* of the system of relations $R^{\delta_1}, \ldots, R^{\delta_m}$ is the relation

$$R^{\delta} = \bigcap_{i=1}^m R^{\delta_i} \times \Sigma^\delta \setminus \delta, \quad \text{where} \quad \delta = \bigcup_{i=1}^m \delta_i.$$  

Let us make two comments for the polynomial case $q = p^n$, where the standard tool for the compatibility analysis is the Gröbner basis method:

- The compatibility condition determined by the *base relation* can be represented by a *single* polynomial, unlike the Gröbner basis, which is normally a system of polynomials.

- Any possible Gröbner basis of polynomials representing the relations $R^{\delta_1}, \ldots, R^{\delta_m}$ corresponds to some combination of consequences of the *base relation*. 

3.1.3. Decomposition of Relations.

If a relation has proper consequences, we can try to express it as far as possible in terms of these consequences, i.e., relations on smaller sets of points. To this end we introduce

**Definition 7** (canonical decomposition). The canonical decomposition of a relation $R^\delta$ with proper consequences $Q^\delta_1, \ldots, Q^\delta_m$ is the relation

$$R^\delta = P^\delta \cap \left( \bigcap_{i=1}^{m} Q^\delta_i \times \Sigma^\delta \text{ \_ \_ \_ \_ \_ \_ \_ \_ \_ \_ \_ \_} \right),$$

(19)

where the factor $P^\delta$ is defined by the following

**Definition 8** (principal factor). The principal factor of the relation $R^\delta$ with proper consequences $Q^\delta_1, \ldots, Q^\delta_m$ is the relation

$$P^\delta = R^\delta \cup \left( \bigcap_{i=1}^{m} Q^\delta_i \times \Sigma^\delta \text{ \_ \_ \_ \_ \_ \_ \_ \_ \_ \_ \_ \_} \right).$$

The principal factor is the maximally “free” — i.e., the closest to the trivial — relation that, together with the proper consequences, makes it possible to recover the initial relation.

If the principal factor in the canonical decomposition is trivial, the relation is completely reduced to relations on smaller sets of points.

**Definition 9** (reducible relation). A relation $R^\delta$ is said to be reducible if it can be represented as

$$R^\delta = \bigcap_{i=1}^{m} Q^\delta_i \times \Sigma^\delta \text{ \_ \_ \_ \_ \_ \_ \_ \_ \_ \_ \_ \_} ,$$

(20)

where $\delta_i$ are proper subsets of $\delta$.

This definition makes it possible to impose a “topology” — i.e., the structure of an abstract simplicial complex with the corresponding theories of homologies, cohomologies, etc. — on an arbitrary $n$-ary relation $R \subseteq \Sigma^n$. This is achieved by

- naming the dimensions of the hypercube $\Sigma^n$ as the “points” $x_1, \ldots, x_n \in X$,
- decomposing $R$ (which can now be denoted by $R^X$) into irreducible components,
- and defining the maximal simplices of the set $\Delta$ as the domains of irreducible components of the relation $R^X$.

3.1.4. On Representation of Relations in Computer.

A few words are needed about computer implementation of relations. To specify a $k$-ary relation $R^k$ we should mark its points within the $k$-dimensional hypercube (or hyperparallelepiped) $\Sigma^k$, i.e., define a characteristic function $\chi : \Sigma^k \rightarrow \{0, 1\}$, with $\chi(\vec{\sigma}) = 1$ or 0 according as $\vec{\sigma} \in R^k$ or $\vec{\sigma} \notin R^k$. Here $\vec{\sigma} = (\sigma_0, \sigma_1, \ldots, \sigma_{k-1})$ is a point of the hypercube. The simplest way to implement the characteristic function is to enumerate all the $q^k$ hypercube points in some standard, e.g., lexicographic order. Then the relation can be represented by a string of $q^k$ bits $\alpha_0 \alpha_1 \cdots \alpha_{q^k-1}$ in accordance with the table:
We call this string *bit table* of relation. Symbolically BitTable \( [i_{\vec{\sigma}}] := (\vec{\sigma} \in R^k) \). Note that \( \vec{\sigma} \) is the (“little-endian”) representation of the number \( i_{\vec{\sigma}} \) in the radix \( q \):

\[
i_{\vec{\sigma}} = \sigma_0 + \sigma_1 q + \cdots + \sigma_i q^i + \cdots + \sigma_{k-1} q^{k-1}.
\]

In the case of hyperparallelepiped \( \Sigma^k = \Sigma_1 \times \Sigma_2 \times \cdots \times \Sigma_k \) one should use the *multi-radix representation* of integers:

\[
i_{\vec{\sigma}} = \sigma_0 + \sigma_1 q_1 + \cdots + \sigma_i q_i \cdots q_1 q_2 \cdots q_{k-1},
\]

where \( 0 \leq \sigma_i < q_{i+1} \), \( i \in [0, \ldots, k - 1] \).

The characteristic function (bit table) can be represented as the binary integer

\[
\chi = \alpha_0 + \alpha_1 2 + \cdots + \alpha_i 2^i + \cdots + \alpha_{q^k-1} 2^{q^k-1}.
\]  

Most manipulations with relations are reduced to very efficient bitwise computer commands. Of course, symmetric or sparse (or, vice versa, dense) relations can be represented in a more economical way, but these are technical details of implementation.

### 3.2. Illustration: Application to Some Cellular Automata

#### 3.2.1. J. Conway’s Game of Life.

The “Life family” is a set of 2-dimensional, binary (i.e., \( \Sigma = \{0, 1\} \); \( q = 2 \)) cellular automata similar to *Conway’s Life*, which rule is defined on 9-cell \((3 \times 3)\) Moore neighborhood and is described as follows. A cell is “born” if it has exactly 3 “alive” neighbors, “survives” if it has 2 or 3 such neighbors, and “dies” otherwise. This rule is symbolized in terms of the “birth”/“survival” lists as B3/S23. Another examples of automata from this family are *HighLife* (the rule B36/S23), and *Day&Night* (the rule B3678/S34678). The site [15] contains collection of more than twenty rules from the Life family with Java applet to run these rules and descriptions of their behavior.

Generalizing this type of local rules, we define a \( k \)-valent *Life rule* as a binary rule on a \( k \)-valent neighborhood (we adopt that \( x_1, \ldots, x_k \) are neighbors of \( x_{k+1} \) of the central cell \( x_{k+1} \)) described by two arbitrary subsets of the set \( \{0, 1, \ldots, k\} \). These subsets \( B, S \subseteq \{0, 1, \ldots, k\} \) contain conditions for the one-time-step transitions \( x_{k+1} \rightarrow x'_{k+1} \) of the forms \( 0 \rightarrow 1 \) and \( 1 \rightarrow 1 \), respectively. Since the number of subsets of any finite set \( A \) is \( 2^{|A|} \) and different pairs \( B/S \) define different rules, the number of different rules defined by two sets \( B \) and \( S \) is equal to \( 2^{k+1} \times 2^k + 1 \). Thus, the total number of \( k \)-valent rules described by the “birth”/“survival” lists is

\[
N_{B/S, k} = 2^{2k+2}.
\]
There is another way to characterize this type of local rules. Let us consider $k$-valent rules symmetric with respect to the group $\text{Sym}(k)$ of all permutations of $k$ outer points of the neighborhood. We shall call such rules $k$-symmetric. It is not difficult to count the total number of different $q$-ary $k$-symmetric rules:

\[ N_{q,\text{Sym}(k)} = q^{(k+q-1)q}. \]  

We see that (23) evaluated at $q=2$ coincides with (22), i.e., $N_{2,\text{Sym}(k)} = N_{B/S,k}$. Since $k$-valent Life rules are obviously $k$-symmetric we have the following

**Proposition.** For any $k$ the set of $k$-symmetric binary rules coincides with the set of $k$-valent Life rules.

This proposition implies in particular that one can always express any $k$-symmetric binary rule in terms of the “birth”/“survival” lists.

The local relation of Conway’s Life automaton $R^\delta_{CL}$ is defined on the 10-set $\delta = \{x_1, \ldots, x_{10}\}$:

Here the point $x_{10} \equiv x'_9$ is the next-time-step of the point $x_9$. By construction, elements of the 10-dimensional hypercube $\Sigma^\delta$ belong to the relation of Conway’s Life automaton, i.e., $(x_1, \ldots, x_{10}) \in R^\delta_{CL}$, in the following cases:

1. \( \left( \sum_{i=1}^{8} x_i = 3 \right) \land (x_{10} = 1), \)
2. \( \left( \sum_{i=1}^{8} x_i = 2 \right) \land (x_9 = x_{10}), \)
3. $x_{10} = 0$, if none of the above conditions holds.

The number of elements of the relation $R^\delta_{CL}$ is $|R^\delta_{CL}| = 512$. The relation $R^\delta_{CL}$, as is the case for any cellular automaton, is functional: the state of $x_{10}$ is uniquely determined by the states of other points. The state set $\Sigma = \{0, 1\}$ can be additionally endowed with the structure of the field $F_2$. We accompany the below analysis of the structure of $R^\delta_{CL}$ by description in terms of polynomials from $F_2 [x_1, \ldots, x_{10}]$. This is done only for illustrative purposes and for comparison with the Gröbner basis method. In fact, we transform the relations into polynomials only for output. Transformation of any relation into polynomial form can be performed by computationally very cheap multivariate version of the Lagrange interpolation. In the case $q=2$, the polynomial which set of zeros corresponds to a relation is constructed uniquely. If $q = p^a > 2$, there is a freedom in the choice of nonzero values of constructed polynomial, and the same relation can be represented by many polynomials.

The polynomial representing $R^\delta_{CL}$ takes the form

\[ P_{CL} = x_{10} + x_9 (\Pi_7 + \Pi_6 + \Pi_3 + \Pi_2) + \Pi_7 + \Pi_3, \]  

(24)
Life the following system of relations (in the polynomial form) that are satisfied for accordance with formula (19). Continuing the decomposition iterations, we finally obtain

Accordingly, the relation seven of them) have the following polynomial form:

One can easily interpret the simplest relations (30): if the point has the form

The above analysis of the relation (19) gives the following: Continuing the decomposition iterations, we finally obtain

where \( \Pi_k \equiv \Pi_k (x_1, \ldots, x_8) \) is the \( k \)th elementary symmetric polynomial defined for \( n \) variables \( x_1, \ldots, x_n \) by the formula:

Hereafter, we will use the following notation:

Applying the computer program to \( R_{CL}^\delta \), we find that the relation \( R_{CL}^\delta \) is reducible and has the decomposition

where \( (i_1, \ldots, i_7) \) is arbitrary 7-element subset of the set \( (1, \ldots, 8) \). For brevity, we dropped in (25) the trivial factors \( \Sigma \{ x_k \} \) entering into the general formula (20).

The eight relations \( R_1^{\delta \{x_i\}} (1 \leq i \leq 8) \) for decomposition (25), it suffices to take any seven of them) have the following polynomial form:

Accordingly, the relation \( R_2^{\delta \{x_9\}} \) has the form

The relations \( R_1^{\delta \{x_i\}} \) and \( R_2^{\delta \{x_9\}} \) are irreducible but not prime, and can be expanded in accordance with formula (19). Continuing the decomposition iterations, we finally obtain the following system of relations (in the polynomial form) that are satisfied for Conway's Life:

One can easily interpret the simplest relations (30): if the point \( x_{10} \) is in the state 1, then at least one point in any set of four points surrounding \( x_9 \) must be in the state 0.

The above analysis of the relation \( R_{CL}^\delta \) takes \( <1 \) sec on a 1.8GHz AMD Athlon notebook with 960Mb.

To compute the Gröbner basis we must add to polynomial (24) ten polynomials

\[ x_i^2 + x_i, \quad i = 1, \ldots, 10 \]

corresponding to the relation \( x^q = x \) that holds for all elements of any finite field \( \mathbb{F}_q \).

Computation of the Gröbner basis over \( \mathbb{F}_2 \) with the help of Maple 9 gives the following:
• pure lexicographic order with variable ordering \( x_{10} \succ x_9 \succ \cdots \succ x_1 \) does not provide any new information leaving initial polynomial (24) unchanged;

• pure lexicographic order with variable ordering \( x_1 \succ x_2 \succ \cdots \succ x_{10} \) reproduces relations (26)—(30) (modulo several polynomial reductions violating the symmetry of polynomials); the computation takes 1 h 22 min;

• degree-reverse-lexicographic order also reproduces system (26)—(30) (same comment as above); the times are: 51 min for the variable ordering \( x_1 \succ x_2 \succ \cdots \succ x_{10} \), and 33 min for the ordering \( x_{10} \succ x_9 \succ \cdots \succ x_1 \).

3.2.2. Elementary Cellular Automata.

Simplest binary, nearest-neighbor, 1-dimensional cellular automata were named elementary cellular automata by S. Wolfram, who has extensively studied their properties [16]. A large collection of results concerning these automata is presented in Wolfram’s online atlas [17]. In the exposition below we use Wolfram’s notations and terminology. The elementary cellular automata are simpler than Conway’s Life, and we may pay more attention to the topological aspects of our approach.

Local rules of the elementary cellular automata are defined on the 4-set \( \delta = \{ p, q, r, s \} \) which can be pictured by the icon \( \begin{array}{c} p \\ q \\ r \\ s \end{array} \). A local rule is a binary function of the form \( s = f(p, q, r) \). There are totally \( 2^{2^3} = 256 \) such functions, each of which can be indexed with an 8-bit binary number.

Our computation with relations representing the local rules shows that the total number 256 of them is divided into 118 reducible and 138 irreducible relations. Only two of the irreducible relations appeared to be prime, namely, the rules 105 and 150 in Wolfram’s numeration. This numeration is based on the “big-endian” — i.e., opposite to our convention (21) — representation of binary numbers. Note, that the prime rules 105 and 150 have linear polynomial forms: \( s = p + q + r + 1 \) and \( s = p + q + r \), respectively.

We consider the elementary automata on a space-time lattice with integer coordinates \( (x, t) \), i.e., \( x \in \mathbb{Z} \) or \( x \in \mathbb{Z}_m \) (spatial \( m \)-periodicity), \( t \in \mathbb{Z} \). We denote a state of the point on the lattice by \( u(x, t) \in \Sigma = \{0, 1\} \). Generally the points are connected as is shown in the picture

![Space-time lattice](image)

The absence of horizontal ties expresses the independence of “space-like” points in cellular automata.

**Reducible Automata.** The analysis shows that some automata with reducible local relations can be represented as unions of automata defined on disconnected subcomplexes:
Two automata 0 and 255 are determined by unary relations $s = 0$ and $s = 1$ on the disconnected set of points:

```
  o o o o o  
  o o o o o  
  o o o o o.  
```

Note that unary relations are usually called *properties*.

Six automata 15, 51, 85, 170, 204 and 240 are, in fact, disjoint collections of spacially zero-dimensional automata, i.e., single cells evolving in time. As an example, let us consider the automaton 15. The local relation is defined on the set $\{p, q, r\}$ and its bit table is 0101010101010101. This relation is reduced to the relation on the face $\{p, r\}$ with bit table 0110. The spacetime lattice is split in the following way:

```
  \begin{array}{c|c|c|c|c|c}
    0 & 0 & 0 & 0 & 1 & 1 \\
    0 & 0 & 0 & 0 & 1 & 1 \\
    1 & 1 & 1 & 1 & 0 & 0 \\
  \end{array}
```

The bit table 0110 means that the points $p$ and $s$ can be only in opposite states, and we can write immediately the general solution for the automaton 15:

$$u(x,t) = a(x-t) + t \mod 2,$$

where $u(x,0) \equiv a(x)$ is an arbitrary initial condition.

Each of the ten automata 5, 10, 80, 90, 95, 160, 165, 175, 245, 250 is decomposed into two identical automata. As an example let us consider the rule 90. This automaton is distinguished as producing the fractal of topological dimension 1 and Hausdorff dimension $\ln 3/\ln 2 \approx 1.58$ known as the *Sierpinski sieve* (or *gasket* or *triangle*). Its local relation on the set $\{p, q, r\}$ is represented by the bit table 1010010101011010. The relation is reduced to the relation with the bit table

```
  10010110  on the face.  (31)
```

It can be seen from the structure of face $\{31\}$ that the spacetime lattice is split into two identical independent complexes as is shown

```
  \begin{array}{c|c|c|c|c|c|c|c|c|c|c|c|c|c}
    1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
  \end{array}
```

```
  \begin{array}{c|c|c|c|c|c|c|c|c|c|c|c|c|c}
    1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
  \end{array}
```

\begin{array}{c}
  \bigcup \\
  \end{array}
To find a general solution of the automaton 90 it is convenient to use the polynomial form of relation (31) \( s + p + r = 0 \). With this linear expression, the general solution is easily constructed:

\[
 u(x, t) = \sum_{k=0}^{t} \binom{t}{k} a(x - t + 2k) \mod 2, \quad u(x, 0) \equiv a(x).
\]

**Using Proper Consequences.** Proper consequences — even if they are not functional — can provide useful information on the behavior of a cellular automaton.

For example, 64 automata \(^\text{10}\) (with both reducible and irreducible local relations) have proper consequences with the bit table

\[
1101
\]

on, at least, one of the faces

\[
\text{\includegraphics[width=5cm]{faces.png}}.
\]

The algebraic forms of relation (32) on faces (33) are \( ps + s = 0, \quad qs + s = 0, \quad rs + s = 0 \), respectively.

Relation (32) is *not functional*, and hence can not describe any deterministic evolution. Nevertheless, it imposes severe restrictions on the behavior of the automata having such proper consequences. The features of the behavior resulting from relation (32) are clearly seen from many of computational results presented in the atlas \[17\]. A typical pattern from this atlas is reproduced in Fig. 3, where several evolutions of the automaton 168 are presented. In the figure, 0’s and 1’s are denoted by the empty and filled square cells,

\[
\text{\includegraphics[width=10cm]{figure3.png}}
\]

Figure 3. Rule 168. Several random initial conditions

respectively. Note that the authors of the figure use a spatially periodic condition: \( x \in \mathbb{Z}_{30} \).

\(^{10}\)The complete list of these automata in Wolfram’s numeration is as follows: 2, 4, 8, 10, 16, 32, 34, 40, 42, 48, 64, 72, 76, 80, 96, 112, 128, 130, 132, 136, 138, 140, 144, 160, 162, 168, 171, 174–176, 186, 187, 190–192, 196, 200, 205, 206, 208, 220, 222–224, 234–239, 241–254.
The local relation of the automaton 168 — its polynomial form is $pqr + qr + pr + s = 0$ — has the proper consequence $rs + s = 0$. Relation (32) means that if, say $r$, as for the rule 168, is in the state 1 then $s$ may be in both states 0 or 1, but if the state of $r$ is 0, then the state of $s$ must be 0:

$$
\begin{align*}
r = 1 & \Rightarrow s = 0 \lor s = 1, \\
r = 0 & \Rightarrow s = 0.
\end{align*}
$$

One can see that all evolutions in Fig. 3 consist of diagonals $x = x_0 - t$ directed leftward and downward. Each diagonal begins with a several units, but after the first appearance of zero all subsequent points along the diagonal are zeros.

**Canonical Decomposition vs. Gröbner Basis.** In this paragraph we compare our canonical decomposition (19) with Gröbner basis in the polynomial case. Let us begin with two examples of elementary cellular automata. The Gröbner bases are computed in the total degree and reverse lexicographical order of monomials. The trivial polynomials $p^2 + p$, $q^2 + q$, $r^2 + r$ and $s^2 + s$ are omitted in the Gröbner bases descriptions.

- **Automaton 30** is remarkable by its chaotic behavior and is even used as a random number generator in Mathematica.

  Relation: 1001010101101010 or $qr + s + r + q + p = 0$.

  **Canonical Decomposition:**

  Proper consequences:

  $$
  \begin{array}{ccc}
  \text{face} & 1 & 2 \\
  \text{bit table} & 11011110 & 11011110 \\
  \text{polynomial} & qs + pq + q & rs + pr + r.
  \end{array}
  $$

  Principal factor: 1011111101111111 or $qrs + pqr + rs + qs + pr + pq + s + p = 0$.

  **Gröbner basis:** \{\(qr + s + r + q + p\), \(qs + pq + q\), \(rs + pr + r\)\}.

  Thus for the rule 30 the polynomials of the canonical decomposition coincide (modulo obvious polynomial substitutions) with the Gröbner basis.

- **Automaton 110** is, like a Turing machine, universal, i.e., it can simulate any computational process, in particular, any other cellular automaton.

  Relation: 1100000100111110 or $pqr + qr + s + r + q = 0$.

  **Canonical Decomposition:**

  Proper consequences:
bit table 11011111 11011111 10010111
polynomial \( pqs + qs + pq + q \)  \( prs + rs + pr + r \)  \( qrs + s + r + q \).

Principal factor: 1111111111111110 or \( pqr s = 0 \).

**Gröbner basis:**

\( \{ prs + rs + pr + r, qs + rs + r + q, qr + rs + s + q, pr + pq + ps \} \).

For automaton 110, the polynomials of the Gröbner basis are not identical with the polynomials of the canonical decomposition. The system of relations defined by the Gröbner basis is:

\[
R_{1}^{\{p,r,s\}} = 11011111 = (prs + rs + pr + r = 0), \\
R_{2}^{\{q,r,s\}} = 10011111 = (qs + rs + r + q = 0), \\
R_{3}^{\{q,r,s\}} = 10110111 = (qr + rs + s + q = 0), \\
R_{4}^{\{p,q,r,s\}} = 110101110111110 = (pr + pq + ps = 0).
\]

In general, the following differences between our approach and the Gröbner basis method can be mentioned.

- In contrast to a Gröbner basis, a base relation, defined as intersection of conditions, agrees with the standard in logic and set theory notion of compatibility.

- In contrast to a canonical decomposition a Gröbner basis may look beyond the polynomial context as a collection of accidental supersets.

- There is some analogy between Gröbner bases and canonical decompositions — in fact, they coincide in about half of cases in our computations.

- Canonical decomposition is more efficient for problems with polynomials of arbitrary degree — the above computation with Conway’s automaton is an example.

- For small degree problems with large number \( n \) of indeterminates the Gröbner basis outperforms canonical decomposition — the number of polynomials of bounded degree is a polynomial function of \( n \), whereas the algorithm of canonical decomposition scans exponential number \( q^n \) of the hypercube points.

4. **Soliton-like Structures in Deterministic Dynamics**

Symmetries of deterministic systems impose severe restrictions on the system dynamics [6]. In particular, for the first order [7] functional relations:

\[ s_t = F(s_{t-1}). \]

\[ ^{11}\text{This means that evolution relation takes the form } s_t = F(s_{t-1}). \]
• dynamical trajectories pass group orbits in non-decreasing order of orbit sizes,

• periodic trajectories lie within orbits of the same size.

One of the characteristic features of dynamical systems with non-trivial symmetries is formation of moving form-preserving structures.

Let us begin with a simple example. Consider a cube $X$ whose vertices take values in two-element set, say $\Sigma = \{0, 1\}$. By the way, as is clear from Fig. 4, a cube can be interpreted as a simplest “finite model of graphene”. The 48-element symmetry group of a cube has the structure $G = \mathbb{Z}_2 \times \text{Sym}(4)$. The group is generated by 3 elements:

1. $120^\circ$ rotation around diagonal of the cube;
2. $90^\circ$ rotation around axis passing through the centers of opposite cube faces;
3. reflection interchanging opposite faces of the cube.

Total number of states of the model is $|\Sigma^X| = 2^8 = 256$. If we assume that the group $\Gamma$ is trivial, then $W = \Gamma^X \rtimes G = 1 \rtimes G \cong G$. The group $W$ splits the set $\Sigma^X$ into 22 orbits in accordance with the table:

| Size of orbits | 1 | 2 | 4 | 6 | 8 | 12 | 24 |
|---------------|---|---|---|---|---|----|----|
| Number of orbits | 2 | 1 | 2 | 5 | 4 | 6 | 6 |

Let us consider a deterministic dynamical system on the cube, namely, symmetric binary 3-valent cellular automaton with the rule 86. The number 86 is the “little endian” representation of the bit string 01101010 taken from the last column of the rule table with $\text{Sym}(3)$-symmetric combinations of values for $x_{1,i}, x_{2,i}, x_{3,i}$

| $x_{1,i}$ | $x_{2,i}$ | $x_{3,i}$ | $x_i$ | $x'_i$ |
|-----------|-----------|-----------|-------|-------|
| 0         | 0         | 0         | 0     | 0     |
| 0         | 0         | 0         | 1     | 1     |
| 1         | 0         | 0         | 0     | 1     |
| 1         | 0         | 0         | 1     | 0     |
| 1         | 1         | 0         | 0     | 1     |
| 1         | 1         | 0         | 1     | 0     |
| 1         | 1         | 1         | 0     | 1     |
| 1         | 1         | 1         | 1     | 0     |
Here $x_i$ is value of $i$th vertex of the cube; $x_{1,i}, x_{2,i}, x_{3,i}$ are values of the cube vertices adjacent to the $i$th one and $x'_i$ is the next time value of $i$th vertex. The rule can also be represented in *Conway's Life* style "Birth"/"Survival" notation as B123/S0, or as polynomial over the field $\mathbb{F}_2$

$$x'_i = x_i + \Pi_3 + \Pi_2 + \Pi_1,$$

where $\Pi_1 = x_{1,i} + x_{2,i} + x_{3,i}$, $\Pi_2 = x_{1,i}x_{2,i} + x_{1,i}x_{3,i} + x_{2,i}x_{3,i}$, $\Pi_3 = x_{1,i}x_{2,i}x_{3,i}$ are elementary symmetric functions.

The phase portrait of the automaton is shown in Fig. 5, where the group orbits are represented by circles containing the ordinal numbers $12$ of orbits within. The numbers over orbits and within cycles are sizes of the orbits (recall that all orbits belonging to the same cycle have equal sizes — see the beginning of this section). The rational number $p$ indicates the weight of the corresponding element of the phase portrait. In fact, $p$ is a probability for randomly chosen state to appear in an isolated cycle or to be caught by an attractor: $p = \frac{\text{size of basin}}{\text{total number of states}}$. Here size of basin is sum of sizes of orbits involved in the struture.

![Figure 5. Rule 86. Equivalence classes of trajectories on hexahedron.](image)

Generalizing this example, we see that if the symmetry group $W$ splits the state set $\Sigma^X$ of deterministic dynamical system into finite number of orbits, then after some lapse of time any trajectory comes inevitably to a cycle over some finite sequence of orbits. This just means formation of soliton-like structures. Namely, let us consider evolution

$$\sigma_{t_0}(x) \rightarrow \sigma_{t_1}(x) = A_{t_1-t_0}(\sigma_{t_0}(x)).$$

(34)

If the states at the moments $t_0$ and $t_1$ belong to the same orbit: $\sigma_{t_0}(x) \in O_i$ and $\sigma_{t_0}(x) \in O_i$, $O_i \subseteq \Sigma^X$; then evolution (34) can be replaced by the group action

$$\sigma_{t_1}(x) = \sigma_{t_0}(x) w, \quad w \in W,$$

These numbers are specified by the computer program in the course of computation.
i.e., the initial state (“shape”) \( \sigma_{t_0}(x) \) is reproduced after some “movement” in the space \( \Sigma^X \).

The following are several examples (including continuous cases) of cycles over group orbits:

- **traveling waves** \( \sigma(x - vt) \) in mathematical physics — the Galilei group;

- **“generalized coherent states”** in quantum physics — unitary representations of compact Lie groups;

- **“spaceships”** in cellular automata — lattice symmetries.

Let us consider the “glider” — one of the “spaceships” in Conway’s Life automaton.

The space \( X \) of Conway’s Life is a square lattice. For the finiteness, we shall assume that the lattice is closed into the \( N \times N \) torus. In the general case \( N \neq 4 \) the symmetry group of \( X \) is the semidirect product of two-dimensional translations \( T^2 = \mathbb{Z}_N \times \mathbb{Z}_N \) and the dihedral group \( D_8 = \mathbb{Z}_4 \rtimes \mathbb{Z}_2 \):

\[
G = T^2 \rtimes D_8, \quad \text{if } N = 3, 5, 6, \ldots, \infty. \tag{35}
\]

In the case \( N = 4 \) the translation subgroup \( T^2 = \mathbb{Z}_4 \times \mathbb{Z}_4 \) is **not normal** and \( G \) has a bit more complicated structure [7]:

\[
\text{normal closure of } T^2 \quad G = \left( ((\mathbb{Z}_2 \times D_8) \rtimes \mathbb{Z}_2) \times \mathbb{Z}_3 \right) \times \mathbb{Z}_2. \tag{36}
\]

The extra symmetry \( \mathbb{Z}_3 \) in (36) can be explained by the \( \mathbb{Z}_3 \) symmetry of the four-vertex Dynkin diagram \( D_4 \) associated with the case \( N = 4 \).

The set of local (cell) states of Conway’s Life is \( \Sigma = \{ \text{“dead”, “alive”} \} = \{ 0, 1 \} \). Since the local rule of Conway’s Life is not symmetric with respect to the transposition \( 0 \leftrightarrow 1 \) of the local states, the internal symmetry group is trivial, i.e., \( \Gamma = \{1\} \) and hence \( \Gamma^X = \{1\} \). Thus, we have \( W = \Gamma^X \rtimes G = 1 \rtimes G \cong G \). The natural action of \( W \) on functions \( \sigma(x) \in \Sigma^X \) takes the form \( \sigma(x)w = \sigma(xg^{-1}) \), where \( w = (1, g) \), \( g \in G \).

Fig. 6 shows four steps of evolution of the glider. The figure demonstrates how the evolution is reduced to the group action. \( N > 4 \) is assumed.

**Figure 6.** Example of soliton-like structure. “Glider” in Conway’s Life is cycle in **two** orbits of the group \( G = T^2 \rtimes D_8 \): configurations \( \sigma_3 \) and \( \sigma_4 \) are obtained from \( \sigma_1 \) and \( \sigma_2 \), respectively, by the same combination of downward **shift**, 90° clockwise **rotation** and **reflection** in respect to vertical.
Comments on Reversibility in Discrete Systems.

A typical deterministic dynamical system is irreversible — it’s phase portrait modulo group orbits looks like in Fig. 5. We see there several isolated and limit cycles (fixed points are regarded as cycles of unit length) accompanied by influxes flowing into the limit cycles. In contrast to continuous systems, any discrete system “forgets” influxes after some time and appears in either isolated or limit cycles. After loss of information about influxes both types of cycles became physically indistinguishable and the system behaves just like reversible. This might be a hint for explanation of observable reversibility of the fundamental laws of nature.

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 horizon — with reversibility and unitarity of the standard quantum mechanics. In several papers of recent years (see, e.g., [18, 19]) ’t Hooft developed an approach to reconciling 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 evolution the limit cycle becomes physically indistinguishable from reversible isolated cycle — the system “forgets” its pre-cycle history.

This type of irreversibility hardly can be observed experimentally (assuming, of course, that considered models may have at all any relation to physical reality). The system should probably spend time of order the Planck unit ($\approx 10^{-44}$ 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.

5. Mesoscopic Lattice Models

Discrete symmetry analysis simplifies manipulations with microcanonical ensembles and search of phase transitions. This allows to reveal subtle details in behavior of mesoscopic models.

5.1. Statistical Mechanics

As we mentioned earlier, 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 is possible with some probability — is a typical example
Analysis of Discrete Dynamical Systems

of non-deterministic dynamical system. In this section we apply symmetry approach to the lattice models in statistical mechanics. These models can be regarded as special instances of Markov chains. Stationary distributions of the 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

\[
Z = \sum_{\sigma \in \Sigma^X} e^{-E_{\sigma}/k_B T}.
\]  

(37)

Here \( \Sigma^X \) is the set of microstates, \( E_{\sigma} \) is energy of microstate \( \sigma \), \( k_B \) is Boltzmann’s constant. The canonical ensemble is 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.

5.2. 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 wide range of applications from nuclei, atomic clusters and nanotechnological structures to multi-star systems [20, 21, 22]. To study mesoscopic systems one should use more fundamental microcanonical ensemble instead of 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

\[
S_E = k_B \ln \Omega_E,
\]  

(38)

or, equivalently, to the microcanonical partition function

\[
\Omega_E = e^{S_E/k_B}.
\]  

(39)

Here \( \Omega_E \) is the number of microstates at fixed energy \( E : \sum E \Omega_E = |\Sigma^X| \). 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, mesoscopic systems demonstrate experimentally and computationally observable 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 point of view of canonical thermostatics — features have natural explanation within microcanonical statistical mechanics [22].

5.2.1. Lattice Models.

In this section we apply 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 subtle details in behavior of system under consideration with the help of exact computation.

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

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

(40)

where $s_i, s_j \in \Sigma$; $J$ is a coupling constant ($J > 0$ and $J < 0$ correspond to ferromagnetic and antiferromagnetic cases, respectively); the first sum runs over all edges $(i, j)$ 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.

Let us remind that if the local symmetry group $G_{\text{loc}}$ decomposes the sets of edges of lattice neighborhoods into nontrivial orbits, then the interaction Hamiltonian should be modified (see, e.g., Eq. (8) on page 9).

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.

Fig. 7 shows microcanonical partition function for the Ising model on the dodecahedron.

Here total number of microstates $|\Sigma^X| = 1048576$, number of lattice vertices $N_X = 20$, energy $E$ is value of Hamiltonian.

Of course, other characteristics of the system can be computed easily in this way.

5.3. 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. Most accepted of them is search of “convex intruders” [23] in the entropy versus energy diagram. In the standard thermodynamics there is a relation

$$\frac{\partial^2 S}{\partial E^2} \bigg|_V = -\frac{1}{T^2} \frac{1}{C_V},$$

(41)

where $C_V$ is the specific heat at constant volume.

Relation (41) implies that $\frac{\partial^2 S}{\partial E^2} \bigg|_V < 0$ and hence the entropy versus energy diagram must be concave. Nevertheless, in mesoscopic systems there might be intervals of
energy where $\frac{\partial^2 S}{\partial E^2} \bigg|_V > 0$. 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, of course, if one accepts that it makes sense to define the variables $T$ and $C_V$ as temperature and the specific heat at these circumstances. In [24] it was demonstrated via computation with exactly solvable lattice models that the convex intruders flatten and disappear in the models with local interactions as the lattice size grows, while in the case of long-range interaction these peculiarities survive even in the limit of an infinite system (both finite and long-range interacting infinite systems are typical cases of systems called nonextensive in statistical mechanics).
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 $\frac{E_{i+1}-E_i}{E_i - E_{i-1}}$ is always rational number $p/q$ and we can write the convexity condition for entropy in terms of numbers of microstates as easily evaluated inequality

$$\Omega_{E_i}^{p+q} < \Omega_{E_{i-1}}^p \Omega_{E_{i+1}}^q.$$  \hfill (42)

As a rule $E_{i+1} - E_i = E_i - E_{i-1}$ and inequality (42) takes the form

$$\Omega_{E_i}^2 < \Omega_{E_{i-1}} \Omega_{E_{i+1}}.$$  

This form means that within convex intruder the number of states with the energy $E_i$ is less than \textit{geometric mean} of numbers of states at the neighboring energy levels.

Fig.\[8\] shows the entropy vs. energy diagram for the Ising model on dodecahedron. The diagram has apparent convex intruder $A$ in the specific energy interval $[-1.2, -0.9]$. Exact computation reveals also a subtle convex intruder $B$ in the interval $[-0.8, -0.6]$.

6. Gauge Connection and Quantization

All most successful contemporary theories in fundamental physics are gauge theories. There are also numerous applications of gauge theories in mathematics (topological quantum field theory, invariants of 3- and 4-manifolds, monoidal categories, Hopf algebras and quantum groups, etc. \cite{25}).

In fact, the gauge principle expresses the very general idea that in spite of the fact that any observable data are represented in different “reference frames” at different points in space\[13\] and time, there should be some way to compare these data.

6.1. Discrete Gauge Principle

At the set-theoretic level, i.e., in the form suitable for both discrete and continuous cases, the main concepts of the gauge principle can be reduced to the following. We have

- a set $\mathcal{T}$, discrete or continuous \textit{time}, $\mathcal{T} \cong \mathbb{Z}$ or $\mathcal{T} \cong \mathbb{R}$;
- a set $X$, \textit{space};
- the sets $\mathcal{T}$ and $X$ are combined into a space-time $\mathcal{M} = X \times \mathcal{T}$;
- a set $\Sigma$, \textit{local states};
- a group $\Gamma \leq \text{Sym}(\Sigma)$ acting on $\Sigma$, \textit{internal symmetries};
- identification of data describing the states from $\Sigma$ makes sense only \textit{modulo} symmetries from $\Gamma$ — this is arbitrariness in the choice of a “\textit{reference frame}”;

\[13\] Consideration only time evolution of general set of states $\mathcal{S}$ leads to the trivial gauge structures. Gauge theories of interest are possible if there exists underlying space structure, i.e., $\mathcal{S} = \Sigma^X$. 
• there is no \textit{a priori} connection between data (i.e., between reference frames) at different points \(x, y \in \mathcal{M}\) — we should impose this connection (or parallel transport) explicitly as \(\Gamma\)-valued function on edges (pairs of points) of abstract graph:

\[
\varsigma(y) = \sigma(x) \pi(x, y), \quad \pi(x, y) \in \Gamma, \quad \sigma(x) \varsigma(y) \in \Sigma;
\]

the connection \(\pi(x, y)\) has the obvious property \(\pi(y, x)^{-1} = \pi(y, x)^{-1}\);

• a connection \(\tilde{\pi}(x, y)\) is called \textit{trivial} if it can be expressed in terms of a function on vertices of the graph: \(\tilde{\pi}(x, y) = p(x)\, p(y)^{-1}, \quad p(x), p(y) \in \Gamma\);

• invariance with respect to the gauge symmetries depending on time and space leads to the transformation rule for connection

\[
\pi(x, y) \rightarrow \gamma(x)^{-1} \pi(x, y) \gamma(y), \quad \gamma(x), \gamma(y) \in \Gamma; \quad (43)
\]

• the curvature of connection \(\pi(x, y)\) is defined as the conjugacy class\footnote{The conjugacy equivalence means that \(\pi(x_1, \ldots, x_k) \sim \gamma^{-1} \pi(x_1, \ldots, x_k) \gamma\) for any \(\gamma \in \Gamma\).} of the holonomy along a cycle of a graph:

\[
\pi(x_1, x_2, \ldots, x_k) = \pi(x_1, x_2) \pi(x_2, x_3) \cdots \pi(x_k, x_1);
\]

the curvature of trivial connection is obviously trivial: \(\tilde{\pi}(x_1, \ldots, x_k) = 1\);

• the gauge principle does not tell us anything about the evolution of the connection itself, so gauge invariant relation describing dynamics of connection (gauge field) should be added.

Let us give two illustrations of how these concepts work in continuous case.

\textbf{Electrodynamics. Abelian prototype of all gauge theories.}

Here the set \(\mathcal{M}\) is 4-dimensional Minkowski space with points \(x = (x^\mu)\) and the set of states is Hilbert space of complex scalar (Schrödinger equation) or spinor (Dirac equation) fields \(\psi(x)\). The symmetry group of the Lagrangians and physical observables is the unitary group \(\Gamma = U(1)\). The elements of \(\Gamma^X\) can be represented as \(e^{-i\alpha(x)}\).

Let us consider the parallel transport for two closely situated space-time points:

\[
\pi(x, x + \Delta x) = e^{-i\rho(x, x + \Delta x)}.
\]

Specializing transformation rule \((43)\) to this particular case

\[
\pi'(x, x + \Delta x) = e^ {i\alpha(x)} \pi(x, x + \Delta x) e^{-i\alpha(x + \Delta x)},
\]

substituting approximations

\[
\pi(x, x + \Delta x) = e^{-i\rho(x, x + \Delta x)} \approx 1 - iA(x)\Delta x,
\]

\[
\pi'(x, x + \Delta x) = e^{-i\rho(x, x + \Delta x)} \approx 1 - iA'(x)\Delta x,
\]
\[ e^{-i\alpha(x+\Delta x)} \approx e^{-i\alpha(x)} (1 - i\nabla\alpha(x)\Delta x), \]

and taking into account commutativity of \( \Gamma = U(1) \) we obtain

\[
A'(x) = A(x) + \nabla\alpha(x) \quad \text{or, in components,} \quad A'_\mu(x) = A_\mu(x) + \frac{\partial\alpha(x)}{\partial x^\mu}. \tag{44}
\]

The 1-form \( A \) taking values in the Lie algebra of \( U(1) \) and its differential \( F = (F_{\mu\nu}) = dA \) are identified with the electromagnetic vector potential and the field strength, respectively. To provide the gauge invariance of the equations for field \( \psi(x) \) we should replace partial by covariant derivatives

\[
\partial_\mu \rightarrow D_\mu = \partial_\mu - iA_\mu(x)
\]

in those equations.

Finally, evolution equations for the gauge field \( A(x) \) should be added. In the case of electromagnetics these are Maxwell’s equations:

\[
d F = 0 \quad \text{first pair} \tag{45}
\]
\[
d * F = 0 \quad \text{second pair.} \tag{46}
\]

Here \( * \) is the Hodge conjugation (Hodge star operator). Note that equation (46) corresponds to vacuum Maxwell’s equations. In the presence of the current \( J \) the second pair takes the form \( * d * F = J \). Note also that the first pair is essentially a priori statement, it reflects simply the fact that \( F \), by definition, is the differential of an exterior form.

**Non-Abelian Gauge Theories in Continuous Space-time.**

Only minor modifications are needed for the case of non-Abelian Lie group \( \Gamma \). Again expansion of the \( \Gamma \)-valued parallel transport for two close space-time points \( x \) and \( x + \Delta x \) with taking into account that \( \pi(x,x) = 1 \) leads to introduction of a Lie algebra valued 1-form \( A = (A_\mu) : \)

\[
\pi(x, x + \Delta x) \approx 1 + A_\mu(x)\Delta x^\mu.
\]

Infinitesimal manipulations with formula (43)

\[
\gamma(x)^{-1}\pi(x, x + \Delta x)\gamma(x + \Delta x) \rightarrow \gamma(x)^{-1}(1 + A_\mu(x)\Delta x^\mu)(\gamma(x) + \frac{\partial\gamma(x)}{\partial x^\mu}\Delta x^\mu)
\]

lead to the following transformation rule

\[
A'_\mu(x) = \gamma(x)^{-1}A_\mu(x)\gamma(x) + \gamma(x)^{-1}\frac{\partial\gamma(x)}{\partial x^\mu}. \tag{47}
\]

The curvature 2-form

\[
F = dA + [A \wedge A]
\]

is interpreted as the physical strength field. In particular, the trivial connection

\[
\tilde{A}_\mu(x) = \gamma_0(x)^{-1}\frac{\partial\gamma_0(x)}{\partial x^\mu}
\]
is flat, i.e., its curvature $F = 0$.

There are different approaches to construct dynamical equations for gauge fields [25]. The most important example is Yang-Mills theory based on the Lagrangian

$$L_{YM} = \text{Tr} \left[ F \wedge \ast F \right].$$

The Yang-Mills equations of motion read

$$dF + [A \wedge F] = 0,$$
$$d \ast F + [A \wedge \ast F] = 0.$$ (48) (49)

Here again equation (48) is a priori statement — the Bianci identity. Note that Maxwell’s equations are a special case of Yang-Mills equations.

It is instructive to see what the Yang-Mills Lagrangian looks like in the discrete approximation. Replacing the Minkowski space $\mathcal{M}$ by a hypercubic lattice one can see that the discrete version of $L_{YM}$ is proportional to $\sum_f \sigma (\gamma_f)$, where the summation is performed over all faces of a hypercubic constituent of the lattice;

$$\sigma = 2 \dim \rho (\Gamma) - \chi (\rho (\Gamma)) - \chi (\rho^\dagger (\Gamma));$$

where $\rho (\Gamma)$ and $\rho^\dagger (\Gamma)$ are fundamental representation of $\Gamma$ and its dual, respectively; $\chi$ is the character; $\gamma_f$ is the gauge group holonomy around the face $f$.

The Yang-Mills theory uses Hodge operation converting $k$-forms to $(n-k)$-forms in $n$-dimensional space with metric $g_{\mu\nu}$. In topological applications so-called BF theory plays an important role since it does not require a metric. In this theory, an additional dynamical field $B$ is introduced. The Lie algebra valued $(n-2)$-form $B$ and the 2-form $F$ are combined into the Lagrangian $L_{BF} = \text{Tr} \left[ B \wedge F \right]$.

6.2. Quantum Behavior and Gauge Connection

The Aharonov–Bohm effect (Fig. 9) is one of the most remarkable illustrations of interplay between quantum behavior and gauge connection. Charged particles moving through the region containing perfectly shielded thin solenoid produce different interference patterns on a screen depending on whether the solenoid is turned on or off. There is no electromagnetic force acting on the particles, but working solenoid produces $U(1)$-connection adding or subtracting phases of the particles and thus changing the interference pattern.

In the discrete time Feynman’s path amplitude [26] is decomposed into the product of elements of the fundamental representation $\rho (\Gamma) = U(1)$ of the circle, i.e., of the Lie group $\Gamma = S^1 = \mathbb{R}/\mathbb{Z}$:

$$A_{U(1)} = \exp (iS) = \exp \left( i \int L dt \right) \rightarrow e^{iL_{0,1}} \ldots e^{iL_{t-1,t}} \ldots e^{iL_{T-1,T}}.$$ (50)

By the notation $L_{t-1,t}$ we emphasize that the Lagrangian is in fact a function defined on pairs of points (graph edges) — this is compatible with physics where the typical Lagrangians are depend on the first order derivatives. Thus we can interpret the expression $\pi (t-1,t) = e^{iL_{t-1,t}} \in \rho (\Gamma) = U(1)$ as $U(1)$-parallel transport.

A natural generalization of this is to suppose that:
Figure 9. Aharonov–Bohm effect. Magnetic flux is confined within the perfectly shielded solenoid; interference pattern is shifted in spite of absence of electromagnetic forces acting on the particles.

- group $\Gamma$ may differ from $S^1$,
- dimension of unitary representation $\rho (\Gamma)$ may differ from 1.

So let us replace expression (50) for Feynman’s path amplitude by the following parallel transport along the path

$$A_{\rho(\Gamma)} = \rho (\alpha_{T,T-1}) \ldots \rho (\alpha_{t,t-1}) \ldots \rho (\alpha_{1,0}).$$

(51)

Here $\alpha_{t,t-1}$ are elements of some group $\Gamma$ — we shall call it quantizing group — and $\rho$ is an unitary representation of $\Gamma$. Note that in (50) the order of factors is not important due to commutativity of $U(1)$. But in (51) we must use the reverse order for consistency with the temporal ordering of non-commutative operators. For discrete and especially finite systems it is natural to take a finite group as the quantizing group, in this case all manipulations — in contrast to the standard quantization — remain within the framework of constructive discrete mathematics requiring no more than the ring of algebraic integers (and sometimes the quotient field of this ring). On the other hand, the standard quantization can be approximated by taking 1-dimensional representations of large enough finite groups.

6.2.1. Illustrative Example Inspired by Free Particle.

In quantum mechanics — as is clear from the never vanishing expression $\exp (\frac{i}{\hbar} S)$ for the path amplitude — transitions from one to any other state are possible in principle. But we shall consider computationally more tractable models with restricted sets of possible transitions.

Let us consider quantization of a free particle moving in one dimension. Such a particle is described by the Lagrangian $L = \frac{m \dot{x}^2}{2}$. Assuming that there are only transitions to the

\[15\]This awkwardness stems from the tradition to write operator actions on the left (cf. footnote 4 on page 4).
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closest points in the discretized space we come to the following rule for the one-time-step transition amplitudes

\[ \begin{align*}
\frac{i}{\hbar} \frac{m(x+1)-x}{2} &= e^{i \frac{m}{2\hbar}} \\
\frac{i}{\hbar} \frac{m(x)-x}{2} &= 1 \\
\frac{i}{\hbar} \frac{m(x-1)-x}{2} &= e^{i \frac{m}{2\hbar}}.
\end{align*} \]

That is, we have evolution rule as an $U(1)$-valued function $R$ defined on pairs of points (graph edges). Symbolically:

\[ R(x \to x) = 1 \in U(1), \]

\[ R(x \to x - 1) = R(x \to x + 1) = w = e^{i \frac{m}{2\hbar}} \in U(1). \tag{52} \]

Now let us assume that $w$ in (52) is an element of some representation of a finite group: $w = \rho(\alpha), \alpha \in \Gamma = \{\gamma_1 = 1, \ldots, \gamma_M\}$. Rearranging multinomial coefficients — trinomial in this concrete case — it is not difficult to write the sum amplitude over all paths from the space-time point $(0, 0)$ to the point $(x, t)$

\[ A^t_x(w) = \sum_{\tau=0}^{t} \frac{\tau!}{(\frac{t-\tau}{2})! \left(\frac{t+\tau}{2}\right)!} \times \frac{t!}{\tau!(t-\tau)!} w^\tau. \tag{53} \]

Note that $x$ must lie in the limits determined by $t$: $x \in [-t, t]$.

One of the most expressive peculiarities of quantum-mechanical behavior is the destructive interference — cancellation of non-zero amplitudes attached to different paths converging to the same point. By construction, the sum of amplitudes in our model is a function $A(w)$ depending on distribution of sources of the particles, their initial phases, gauge fields acting along the paths, restrictions — like, e.g., “slits” — imposed on possible paths, etc. In the case of 1-dimensional representation the function $A(w)$ is a polynomial with algebraic integer coefficients and $w$ is a root of unity. Thus the condition for destructive interference can be expressed by the system of polynomial equations: $A(w) = 0$ and $w^M = 1$. For concreteness let us consider the cyclic group $\Gamma = \mathbb{Z}_M = \{\gamma_1, \ldots, \gamma_k, \ldots, \gamma_M\}$. Any of its $M$ irreducible representations takes the form $\rho(\gamma_k) = w^{k-1}$, where $w$ is one of the $M$th roots of unity. For simplicity let $w$ be the primitive root: $w = e^{2\pi i/M}$.

Fig. 10 shows all possible transitions (with their amplitudes) from the point $x$ in three time steps. We see that the polynomial $A^3_x(w) = 3w + 3w^3 = 3w^2 + 1 = \Phi_4(w)$ contains the cyclotomic polynomial $\Phi_4(w) = w^2 + 1$ as a factor. The smallest group associated to $\Phi_4(w)$ — and hence providing the destructive interference — is $\mathbb{Z}_4$, which we shall consider as quantizing group for the model.

Fig. 11 shows interference patterns — normalized squared amplitudes (“probabilities”) — from two sources placed in the positions $x = -4$ and $x = 4$ for 20 time steps. The upper and lower graph show interference pattern when sources are in the same ($\Delta \phi = 0$) and in the opposite ($\Delta \phi = \pi$) phases, respectively.
6.2.2. Local Quantum Models on Regular Graphs.

The above model — with quantum transitions allowed only within the neighborhood of a vertex of a 1-dimensional lattice — can easily be generalized to arbitrary regular graph. Our definition of local quantum model on k-valent graph includes the following:

1. *Space* $X = \{x_1, \ldots, x_{N_X}\}$ is a $k-$valent graph.

2. *Set of local transitions* $E_i = \{e_{0,i}, e_{1,i}, \ldots, e_{k,i}\}$ is the set of $k$ adjacent to the vertex $x_i$ edges $e_{m,i} = (x_i \to x_{m,i})$ completed by the edge $e_{0,i} = (x_i \to x_i)$.

3. We assume that the *space symmetry* group $G = \text{Aut}(X)$ acts transitively on the set \{E_1, \ldots, E_{N_X}\}.

4. $G_{\text{loc}} = \text{Stab}_G(x_i) \leq G$ is the stabilizer of $x_i$.

5. $\Omega_i = \{\omega_{0,i}, \omega_{1,i}, \ldots, \omega_{h,i}\}$ is the set of orbits of $G_{\text{loc}}$ on $E_i$.

6. *Quantizing group* $\Gamma$ is a finite group: $\Gamma = \{\gamma_1, \ldots, \gamma_M\}$. 
7. **Evolution rule** $R$ is a function on $E_i$ with values in some representation $\rho(\Gamma)$. The rule $R$ prescribes $\rho(\Gamma)$-weights to the one-time-step transitions from $x_i$ to elements of the neighborhood of $x_i$. From the symmetry considerations $R$ must be a function on orbits from $\Omega_i$, i.e., $R(e_{m,i}g) = R(e_{m,i})$ for $g \in G_{loc}$.

To illustrate these constructions, let us consider the local quantum model on the graph of **buckyball** (see detailed consideration of this graph at page 8). Here the space $X = \{x_1, \cdots, x_{60}\}$ has the symmetry group $G = \text{Aut}(X) = \mathbb{Z}_2 \times \text{Alt}(5)$. The set of local transitions takes the form $E_i = \{e_{0,i}, e_{1,i}, e_{2,i}, e_{3,i}\}$, where
\[
\begin{align*}
  e_{0,i} &= (x_i \rightarrow x_i), \\
  e_{1,i} &= (x_i \rightarrow x_{1,i}), \\
  e_{2,i} &= (x_i \rightarrow x_{2,i}), \\
  e_{3,i} &= (x_i \rightarrow x_{3,i}).
\end{align*}
\]
The stabilizer of $x_i$ is $G_{loc} = \text{Stab}_G(x_i) = \mathbb{Z}_2$. The set of orbits of $G_{loc}$ on $E_i$ contains 3 orbits:
\[
\Omega_i = \{\omega_{0,i} = \{e_{0,i}\}, \omega_{1,i} = \{e_{1,i}, e_{2,i}\}, \omega_{2,i} = \{e_{3,i}\}\},
\]
i.e., the stabilizer does not move the edges $(x_i \rightarrow x_i)$ and $(x_i \rightarrow x_{3,i})$ and swaps $(x_i \rightarrow x_{1,i})$ and $(x_i \rightarrow x_{2,i})$.

The evolution rule takes the form:
\[
\begin{align*}
  R(x_i \rightarrow x_i) &= \rho(\alpha_0), \\
  R(x_i \rightarrow x_{1,i}) &= R(x_i \rightarrow x_{2,i}) = \rho(\alpha_1), \\
  R(x_i \rightarrow x_{3,i}) &= \rho(\alpha_2),
\end{align*}
\]
where $\alpha_0, \alpha_1, \alpha_2 \in \Gamma$. If we take a 1-dimensional representation and move $\alpha_0$ — using gauge invariance — to the identity element of $\Gamma$, we see that the rule $R$ depends on two elements $v = \rho(\alpha_1)$ and $w = \rho(\alpha_2)$. Thus the amplitudes in the quantum model on the buckyball take the form $A(v, w)$ depending on two roots of unity. To search nontrivial quantizing groups one should check (by, e.g., Gröbner basis computation) compatibility of the system of polynomial equations $A(v, w) = \Phi_i(v) = \Phi_j(w) = 0$, where $\Phi_i(v)$ and $\Phi_j(w)$ are cyclotomic polynomials.

### 6.3. General Discussion of Quantization in Finite Systems

As is well known, Feynman’s approach is equivalent to the traditional matrix formulation of quantum mechanics, where the time evolution $|\psi_0\rangle \rightarrow |\psi_T\rangle$ of a system from the initial state vector to the final is described by the evolution matrix $U$: $|\psi_T\rangle = U |\psi_0\rangle$. The evolution matrix can be represented as the product of matrices corresponding to the single time steps: $U = U_{T_{e-T-1}} \cdots U_{t_{t-1}} \cdots U_{1_{e-0}}$. In fact, Feynman’s quantization — i.e., the rules “multiply subsequent events” and “sum up alternative histories” — is simply a rephrasing of matrix multiplication. This is clear from the below illustration presenting two-time-step evolution of a two-state system (single qubit) in both Feynman’s and matrix forms — the general case of many time steps and many states can easily be obtained (by induction for example).
We see that in accordance with Feynman’s rules the transition from, e.g., $\phi_2$ to $\psi_1$ is determined by the expression $b_{11}a_{12} + b_{12}a_{22}$. But this is just the element $u_{12}$ of the matrix product $U = BA$ performing evolution $|\psi\rangle = U|\phi\rangle$, where $|\phi\rangle = \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix}$ and $|\psi\rangle = \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$.

Of course, such reduction of sums over histories to matrices is applicable to the case of transitions along paths being gauge connections as in (51). In this case matrix elements of an $N_X \times N_X$ evolution matrix $U$ are themselves matrices from the representation $\rho(\Gamma)$. We can ignore this particular block structure of the matrix and consider $U$ as an $N \times N$ matrix over the field $\mathbb{C}$, where $N = N_X \times \dim \rho(\Gamma)$.

In quantum mechanics, the evolution matrices $U$ are unitary operators acting in Hilbert spaces of state vectors (called also “wave functions”, “amplitudes” etc.). Quantum mechanical particles are associated with unitary representations of some groups. According to their dimensions, these representations are called “singlets”, “doublets”, etc. Multidimensional representations describe the spin. A quantum mechanical experiment is reduced to comparison of the system state vector $|\psi\rangle$ with some sample state vector $|\phi\rangle$. According to the Born rule, the probability to observe coincidence of the states is equal to $|\langle \phi | \psi \rangle|^2$, where $\langle \cdot | \cdot \rangle$ is the inner product in the Hilbert space. To see what these constructions may look like in the constructive finite background, let us assume that evolution operators are elements of a representation of a finite group.

### 6.3.1. Permutations and Linear Representations

Having a finite group $G = \{e_1 = 1, \ldots, e_m\}$, we can easily describe all its transitive actions on finite sets [27]. Any such set $\Omega = \{\omega_1, \ldots, \omega_n\}$ is in one-to-one correspondence with the right (or left) cosets of some subgroup $H \leq G$, i.e., $\Omega \cong H \backslash G$ (or $G/H$) is the homogeneous space (or $G$-space). Action of $G$ on $\Omega$ is faithful if the subgroup $H$ does not contain normal subgroups of $G$. We can write actions in terms of permutations

$$\pi(g) = \begin{pmatrix} \omega_i \\ \omega_j \end{pmatrix} \sim \begin{pmatrix} Ha \\ Hag \end{pmatrix}, \quad g, a \in G, \quad i, j = 1, \ldots, n.$$  

Maximum transitive set $\Omega$ is the group itself, i.e., in the above construction $H = \{1\}$. The action on $\Omega = G$ is called regular and can be represented by permutations

$$\Pi(g) = \begin{pmatrix} e_i \\ e_i g \end{pmatrix}, \quad i = 1, \ldots, m.$$  

(54)
To introduce “numerical” (“statistical”) description, let us assume that \( \omega_i \)'s are basis elements of a linear vector space \( \mathcal{H} \) over a field \( F \)

\[
\mathcal{H} = \text{Span} (\omega_1, \cdots, \omega_n),
\]

i.e., we prescribe \( F \)-valued “weights” to the elements \( \omega_i \in \Omega \). Then we can write permutations in the matrix form:

\[
\pi(g) \rightarrow \rho(g) = [\rho(g)_{ij}], \quad \text{where} \quad \rho(g)_{ij} = \delta_{\omega_i g, \omega_j}; \quad i, j = 1, \ldots, n; \quad (56)
\]

\[
\delta_{\alpha,\beta} \equiv \begin{cases} 
1, & \text{if } \alpha = \beta, \\
0, & \text{if } \alpha \neq \beta 
\end{cases} \quad \text{for } \alpha, \beta \in \Omega.
\]

The so defined function \( \rho \) is called a permutation representation. The matrix form of \((54)\)

\[
\Pi(g) \rightarrow P(g) = [P(g)_{ij}], \quad P(g)_{ij} = \delta_{e_i g, e_j}, \quad i, j = 1, \ldots, m \quad (57)
\]

is called the regular representation. It is assumed that \( F \) is an algebraically closed field — usually the field of complex numbers \( \mathbb{C} \). But in the case of finite groups the quotient field of the ring \( \Lambda \) of algebraic integers\(^{16} \) is sufficient for all reasonable purposes — \( \Lambda \) is a constructive subset of \( \mathbb{C} \).

Let us recall some relevant background information about linear representations of finite groups \([28]\).

1. Any linear representation of a finite group \( G \) is unitary since there is always an unique invariant inner product \( \langle \cdot | \cdot \rangle \) making any space of representation \( \mathcal{H} \) into a Hilbert space.

2. All possible irreducible unitary representations of the group \( G \) are contained in the regular representation \((57)\). More specifically, all matrices \((57)\) can simultaneously be reduced by some unitary transformation \( S \) to the form

\[
S^{-1}P(g)S = \begin{bmatrix}
\Delta_1(g) \\
d_2 \begin{bmatrix}
\Delta_2(g) \\
\ddots \\
\Delta_2(g)
\end{bmatrix} \\
\ddots \\
\end{bmatrix}.
\]

\[
\Delta_r(g)
\]

\[
S^{-1}P(g)S = \begin{bmatrix}
\Delta_1(g) \\
d_2 \begin{bmatrix}
\Delta_2(g) \\
\ddots \\
\Delta_2(g)
\end{bmatrix} \\
\ddots \\
\end{bmatrix}.
\]

Here \( r \) is the number of different irreducible representations \( \Delta_j \) of the group \( G \). This number coincides with the number of conjugacy classes\(^{17} \) in \( G \). The number \( d_j \) is

---

\(^{16}\)The ring of algebraic integers consists of the roots of monic polynomials with integer coefficients. A polynomial is called monic if its leading coefficient is unit.

\(^{17}\)The \( j \)th conjugacy class \( C_j \subseteq G \) consists of all group elements of the form \( g^{-1} c_j g \), where \( c_j \in C_j \) is some (arbitrary) representative of the class, \( g \in G \), \( j = 1, \ldots, r \).
simultaneously the dimension of $\Delta_j$ and its multiplicity in the regular representation, so it is obvious that $d_1^2 + d_2^2 + \cdots + d_r^2 = |G| = m$. It can be proved also that any $d_j$ divides the number of elements of $G$: $d_j \mid m$.

3. Any irreducible representation $\Delta_j$ is determined uniquely (up to isomorphism) by its character $\chi_j$. The character is a function on $G$ defined as $\chi_j(a) = \text{Tr} \Delta_j(a)$, $a \in G$. The character is a central or class function, i.e., it is constant on the conjugacy classes: $\chi_j(a) = \chi_j(g^{-1}ag)$, $a, g \in G$. Any class function $\varphi(a)$ on $G$ is a linear combination of the characters $\chi_1, \ldots, \chi_r$.

4. All values of $\chi_j$ and eigenvalues of $\Delta_j$ are elements of the ring $\mathbb{A}$ of algebraic integers, moreover the eigenvalues are roots of unity.

5. A convenient form of describing all irreducible representation of a finite group $G$ is the character table. The columns of this table correspond to the conjugacy classes of $G$ while its rows correspond to the characters $\chi_j$ of the inequivalent irreducible representations of $G$.

|          | $1$   | $c_2$ | $\cdots$ | $c_r$ |
|----------|-------|-------|-----------|-------|
| $\chi_1$| 1     | 1     | $\cdots$ | 1     |
| $\chi_2$| $\chi_2(c_1)$ | $\chi_2(c_2)$ | $\cdots$ | $\chi_2(c_r)$ |
| $\vdots$| $\vdots$ | $\vdots$ | $\cdots$ | $\vdots$ |
| $\chi_r$| $\chi_r(c_1)$ | $\chi_r(c_2)$ | $\cdots$ | $\chi_r(c_r)$ |

The $j$th column is indicated by a representative $c_j \in C_j$ of the $j$th conjugacy class $C_j$. Conventionally we take $c_1 = 1$ and $\chi_1$ to be the trivial character corresponding to the trivial 1-dimensional representation.

### 6.3.2. Interpretation of Quantum Description in Finite Background

Let us discuss sketchy (more detailed presentation see in [29]) constructive approach to the interpretation of quantum description.

Summarizing the above, we see that dynamics of finite quantum model of any type is reduced ultimately to a single finite-dimensional unitary $k \times k$ matrix $U$ describing transitions between initial and final vectors in some $k$-dimensional Hilbert space $H_k$. In the finite background the matrix $U$ is an element of unitary representation $\Delta$ of a finite group $G$, i.e., the number of all possible evolutions is equal to $m = |G|$. We shall assume, as is accepted in quantum mechanics, that $\Delta$ is direct sum of irreducible representations $\Delta_j$ from (58).

The decomposition of the Hilbert space into irreducible components is an important part of the mathematical formulation of quantum mechanics. Such dependence on the choice of the basis in the Hilbert space may seem unusual for a physical theory. But, in fact, a basis in which the Hilbert space is reduced — we shall call such a basis quantum basis — simply reflects the structure of underlying symmetry group.

We can construct a $G$-space $\Omega = \{\omega_1, \ldots, \omega_n\}$ in such a way that its permutation representation (56) contains $\Delta$ as subrepresentation (obviously $n \geq k$). That is, the space

---

In the case that $\Delta$ is reducible representation, the set $\Omega$ may be intransitive union of transitive $G$-spaces.
$H_k$ is subspace of the Hilbert space $H_n$ of the permutation representation. We shall call the basis $\{\omega_1, \ldots, \omega_n\}$ in the space $H_n$ the permutation basis. Transitions from the permutation to quantum basis for matrices $\tilde{U}$ and vectors $|\tilde{\psi}\rangle \in H_n$ are given by the formulas

$$
\tilde{U}_q = S^{-1} U_p S, \quad (59)
$$

$$
|\tilde{\psi}_q\rangle = S^{-1} |\tilde{\psi}_p\rangle. \quad (60)
$$

Now we can embed any evolution $U$ with the matrix $\Delta$ in the space $H_k$ into the evolution $\tilde{U}$ in the space $H_n$. In the quantum basis the matrix of $\tilde{U}$ takes the form

$$
\tilde{U}_q = \begin{bmatrix} \Delta & 0 \\ 0 & A \end{bmatrix}, \quad (61)
$$

where $A$ is an $(n-k) \times (n-k)$ matrix. Due to the form of (61) the evolution $U$ described by $\Delta$ is completely independent of the components of vectors of $H_n$ related to $A$. The “hidden variables” that can come from the additional components describe degrees of freedom reflecting indistinguishability of $\omega_i$’s lying in the same group orbit. The evolution $\tilde{U}$ is simply a permutation of $\omega_i$’s and can not manifest anything quantum.

**Illustration.** A quantum model with the group $\text{Sym}(3)$. The group $G = \text{Sym}(3)$ is the group of all permutations of three objects. This is the smallest non-commutative group. Its 6 elements form the following 3 conjugate classes $C_1 = \{1 = ()\}, C_2 = \{a_1 = (12), a_2 = (23), a_3 = (13)\}, C_3 = \{b_1 = (123), b_2 = (132)\}$. We used here the cyclic notation for permutations. The group has three nonequivalent irreducible representations described by the character table

$$
\begin{array}{ccc}
\chi_1 & 1 & 1 & 1 \\
\chi_2 & 1 & -1 & 1 \\
\chi_3 & 2 & 0 & -1 \\
\end{array}
$$

Let us take for example the 2-dimensional representation $\Delta$ with the character $\chi_3$. The representation is given by the following set of $2 \times 2$ matrices:

$$
\Delta(1) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},
\Delta(a_1) = \begin{bmatrix} 0 & e^{-2\pi i/3} \\ e^{2\pi i/3} & 0 \end{bmatrix}, \quad \Delta(a_2) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \Delta(a_3) = \begin{bmatrix} 0 & e^{2\pi i/3} \\ e^{-2\pi i/3} & 0 \end{bmatrix},
\Delta(b_1) = \begin{bmatrix} e^{2\pi i/3} & 0 \\ 0 & e^{-2\pi i/3} \end{bmatrix}, \quad \Delta(b_2) = \begin{bmatrix} e^{-2\pi i/3} & 0 \\ 0 & e^{2\pi i/3} \end{bmatrix}.
$$

The regular permutation representation of $\text{Sym}(3)$ is 6-dimensional. But 3-dimensional faithful permutation representation induced by the action on the homogeneous space $\text{Sym}(2) \setminus \text{Sym}(3) \cong \Omega = \{\omega_1, \omega_2, \omega_3\}$ also contains $\Delta$. Since any permutation representation contains trivial 1-dimension subrepresentation, the only possible choice of the addition $A$ is the representation corresponding to the first row of the above character table. Thus, for $\tilde{U}_q$ we have
The most general unitary matrix of transition from the permutation to the quantum basis takes the form

\[
S = \frac{e^{\alpha i}}{\sqrt{3}} \begin{bmatrix}
1 & e^{2\pi i/3} & e^{\beta i} \\
e^{\pi i/3} & e^{-2\pi i/3} & e^{\beta i} \\
e^{-2\pi i/3} & e^{2\pi i/3} & e^{\beta i}
\end{bmatrix}, \quad \text{where } \alpha, \beta \text{ are arbitrary real parameters.}
\] (62)

Any quantum evolution of the form \( |\psi\rangle = U |\phi\rangle \), where \( |\phi\rangle = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} \) and \( |\psi\rangle = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix} \), \( U \) is one of the matrices \( \Delta \); can be extended to the evolution \( |\tilde{\psi}_q\rangle = U_q |\tilde{\phi}_q\rangle \), where

\[
|\tilde{\phi}_q\rangle = \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} \text{ and } |\tilde{\psi}_q\rangle = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{bmatrix}, \quad \phi_3 \text{ is arbitrary additional component.}
\]

Then, applying the transformation \( S \), we come to the classical evolution with the matrix \( \tilde{U}_p = S U_q S^{-1} \) which simply permutes the components of the initial vector

\[
|\tilde{\phi}_p\rangle = S |\tilde{\phi}_q\rangle = \frac{e^{\alpha i}}{\sqrt{3}} \begin{bmatrix}
e^{2\pi i/3} \phi_1 + e^{\beta i} \phi_3 \\
e^{2\pi i/3} \phi_1 + e^{\beta i} \phi_3 \\
e^{2\pi i/3} \phi_1 + e^{\beta i} \phi_3 
\end{bmatrix}
\]

without performing any algebraic manipulations with the components.
7. Conclusion

In this chapter we discuss the general concept of discrete dynamical system and its specialization involving underlying space structures. We apply various constructive approaches to study discrete and finite dynamical systems.

We construct a family of groups unifying space and internal symmetries in a natural way. This construction generalizes the standard direct and wreath products.

We introduce the concept of a system of discrete relations on an abstract simplicial complex. This system can be treated as a natural generalization of cellular automata or as a set-theoretical analog of systems of polynomial equations.

We developed and implemented algorithms for analyzing compatibility of systems of discrete relations and for constructing canonical decompositions of discrete relations.

Applying the technique described above to some cellular automata — a particular case of discrete relations — we obtained a number of results. The most interesting among them, in our opinion, is the demonstration of how the presence of non-trivial proper consequences may determine the global behavior of an automaton.

We suggest an algorithmic approach — based on discrete symmetry analysis and implemented in C — for construction and investigation of discrete dynamical models — deterministic, mesoscopic and quantum. We hope that our approach can be used in various practical applications, such as, for example, simulation of nanostructures with nontrivial symmetry properties.

We demonstrate that soliton-like moving structures — like “spaceships” in cellular automata, “traveling waves” in mathematical physics and “generalized coherent states” in quantum physics — arise inevitably in deterministic dynamical systems whose symmetry group splits the set of states into finite number of group orbits.

We formulate the gauge principle in the form most suitable for discrete and finite systems. We also propose a method — based on introduction of unitary gauge connection of a special kind — for quantizing discrete systems and construct simple models for studying properties of suggested quantization.

We show that if unitary operators describing dynamics of finite quantum system form finite group, then the system can be embedded into a classical system with a simple behavior. We hope that discrete and finite background allowing comprehensive study may lead to deeper understanding of the quantum behavior and its connection with symmetries of systems.

To study more complicated models we are developing C programs based on computer algebra and computational group theory methods.

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