Symmetries and Dynamics of Discrete Systems

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Motivations

- Symmetry analysis of finite discrete systems can be complete in contrast to continuous systems where only negligible small part of all thinkable symmetries is considered: point and contact Lie, Bäcklund and Lie–Bäcklund, sporadic instances of non-local symmetries etc.

- Many hints from quantum mechanics and quantum gravity that discreteness is more suitable for physics at small distances than continuity which arises only as a logical limit in considering large collections of discrete structures.
Any collection of discrete points taking values in finite sets possesses some kind of locality:
such collection has a structure of abstract simplicial complex
Special cases are
- systems of polynomial equations over finite fields
- cellular automata

In this talk we consider relations on graphs — 1D simplicial complexes

Two types of discrete dynamical systems — discrete relations evolving in discrete time:
- state of deterministic system at any point of time is function of previous states (we consider cellular automata with symmetric local rules)
- in non-deterministic system transition from one state to any other state is possible with some probability (we consider mesoscopic lattice models — some ensembles of discrete relations)
Space of discrete dynamical system is lattice $\Gamma \equiv k$-valent graph
Symmetry of lattice $\Gamma$ is graph automorphism group $\text{Aut}(\Gamma)$
We assume $\text{Aut}(\Gamma)$ acts transitively on vertices $V(\Gamma)$ of lattice: very idea of “space” implies possibility to reach any point by “moves” in the space

In applications it is assumed often that lattice is embedded in some continuous space — in this case notion of ‘dimension’ of lattice makes sense
In our context such embeddings are of little importance — we shall use them for visualization only
Functions on Lattices and Their Orbits

- $Q = \{0, \ldots, q - 1\}$ is set of values of lattice vertices
- $\Sigma = Q^\Gamma$ is space of $Q$-valued functions on $\Gamma$
- $\text{Aut}(\Gamma)$ acts non-transitively on $\Sigma$ splitting this space into orbits of different sizes $\Sigma = \bigcup_{i=1}^{N_{\text{orbits}}} O_i$

Action: $(g\varphi)(x) = \varphi(g^{-1}x)$

$x \in V(\Gamma), \varphi(x) \in \Sigma, g \in \text{Aut}(\Gamma)$

- Burnside’s lemma counts total number of orbits

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

$N_{\text{cycles}}^g$ is number of cycles in group element $g$
Examples of Lattices

- Tetrahedron
- Hexahedron (= Graphene $4 \times 2$)
- Icosahedron
- Dodecahedron

Graphene $6 \times 4$
Triangular $4 \times 6$
Square $5 \times 5$
Buckyball

V. V. Kornyak (LIT, JINR)
Cube Is “Smallest Graphene” (Graphene $4 \times 2$)

Embeddings of graph of Hexahedron form

4-gonal (6 tetragons) regular tiling of sphere $S^2$ and
6-gonal (4 hexagons) regular tiling of torus $T^2$
Some Quantitative Characteristics
of lattices, their groups and orbits

| Lattice            | $|V(\Gamma)|$ | $|\text{Aut}(\Gamma)|$ | $\Omega = q^{|V(\Gamma)|}$ | $N_{\text{orbits}}$ |
|--------------------|---------------|-------------------------|-----------------------------|---------------------|
| Tetrahedron        | 4             | 24                      | 16                          | 5                   |
| Hexahedron         | 8             | 48                      | 256                         | 22                  |
| Icosahedron        | 12            | 120                     | 4096                        | 82                  |
| Dodecahedron       | 20            | 120                     | 1048576                     | 9436                |
| Graphene $6 \times 4$ Torus | 24         | 48                      | 16777216                    | 355353              |
| Graphene $6 \times 4$ Klein bottle | 24         | 16                      | 16777216                    | 1054756             |
| Triangular $4 \times 6$ | 24         | 96                      | 16777216                    | 180070              |
| Square $5 \times 5$  | 25            | 200                     | 33554432                    | 172112              |
| Buckyball          | 60            | 120                     | $1152921504606846976 \approx 10^{18}$ | $9607679885269312 \approx 10^{16}$ |

Klein bottle arrangement is non-transitive (2 orbits of sizes 8 and 16)
We discard such graphs as counterintuitive nonhomogeneous spaces
C Program

Input

- **Graph** $\Gamma = \{N_1, \ldots, N_n\}$
  - $N_i$ is neighborhood of $i$th vertex
- **Cellular automata branch:**
  - Set of local rules $R = \{r_1, \ldots, r_m\}$
  - $r_i$ is bit representation of $i$th rule
- **Lattice model branch:**
  - Hamiltonian of the model
- **Control parameters**
Program produces

- **automorphism group** $\text{Aut}(\Gamma)$
- **Cellular automata branch:**
  - phase portraits of automata modulo $\text{Aut}(\Gamma)$ for all rules from $R$
  - Manipulating control parameters we can
    - select automata with specified properties, e.g., reversibility, Hamiltonian conservation etc.
    - search automata producing specified structures, e.g., limit cycles, isolated cycles, “Gardens of Eden”, “Spaceships” etc.
- **Lattice model branch:**
  - partition function and other characteristics of the model
  - search of phase transitions
General Dynamical Principle Induced By Symmetry

For Any Deterministic Dynamical System

- trajectories can be directed only from larger orbits to smaller orbits or to orbits of the same size
- periodic trajectories must lie within the orbits of equal size

Meaning: any isolated system may only lose information in its evolution — analog of “Second Law of Thermodynamics”

Simple consequence of the fact that “deterministic” means “functional”
Group Origin of Emergent Structures: typical phase portrait modulo $\text{Aut}(\Gamma)$ contains soliton-like structures — “spaceships”
Eventually (Part of) Dynamics Is Reduced To Group Actions

State \( \varphi(x) \in O_i \) in cycle starting at moment 0 evolves after some time \( t \) into state \( \varphi_t(x) = A_t(\varphi(x)) \) in the same orbit \( O_i \).

Hence:

Evolution operator \( A_t \) can be replaced by group action

\[
\varphi_t(x) = A_t(\varphi(x)) = \varphi(g_t^{-1}x)
\]

i.e., initial shape \( \varphi(x) \) is reproduced via some movement in space — formation of soliton-like structure.

Galilei group analogy: many equations of mathematical physics have running wave solutions \( \varphi(x - vt) \) \( = \varphi(g_t^{-1}x) \) for Galilei group.
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Symmetries of Toric $N \times N$ Square Lattices $\Gamma_{N \times N}$

$\Gamma_{N \times N}$ has the same group $G_{N \times N}$ in both 4-valent von Neumann and 8-valent Moore cases.

### Principal case

$N = 3, 5, 6, \ldots, \infty$  \hspace{0.5cm} $|G_{N \times N}| = 8N^2$  \hspace{0.5cm} $T^2$ is normal

$G_{N \times N} = T^2 \rtimes D_4$ — semidirect product of $T^2$ and $D_4$

$T^2 = \mathbb{Z}_N \times \mathbb{Z}_N$ — translation group ($\mathbb{Z}_\infty \equiv \mathbb{Z}$)

$D_4 = \mathbb{Z}_4 \rtimes \mathbb{Z}_2$ — dihedral group ($\mathbb{Z}_4$ – 90° rotations, $\mathbb{Z}_2$ – reflections)

Resembles Euclidean group $E_2 = (T^2 = \mathbb{R} \times \mathbb{R}) \rtimes O(2)$

### Exception: $N = 4$

$|G_{4 \times 4}| = 3 \times 8N^2$  \hspace{0.5cm} $T^2$ is not normal

Normal closure of $T^2$

$G_{4 \times 4} = (((((\mathbb{Z}_2 \times D_4) \times \mathbb{Z}_2) \times \mathbb{Z}_3) \times \mathbb{Z}_2) \times \mathbb{Z}_2) \times \mathbb{Z}_2$ (by GAP algorithm)
Group Interpretation of “Glider”

Evolution operator = group action: \( \varphi_{tb}(x) = A_{ta tb} (\varphi_{ta}(x)) = \varphi_{ta} \left(g_{ta tb}^{-1} x \right) \)

One step diagonal shift

\( g_{15} \in T^2 \)

“Glider” over translation group \( T^2 \) is cycle in 4 orbits

One step downward shift \( \rightarrow 90^\circ \) clockwise rotation \( \rightarrow \) reflection in respect to vertical

\( g_{13} = g_{24} \in T^2 \rtimes D_4 \)

“Glider” over maximal symmetry group \( T^2 \rtimes D_4 \) is cycle in 2 orbits
Two Examples of Trivalent Cellular Automata with Symmetric Local Rules

- Rule 86 = 01101010 \sim \text{B123/S0} \sim x'_4 = x_4 + \sigma_3 + \sigma_2 + \sigma_1

- Rule 23 = 11101000 \sim \text{B012/S0} \sim x'_4 = x_4(\sigma_2 + \sigma_1) + \sigma_3 + 1

Rule 23 is BW symmetric

Notations: \sigma_1 = x_1 + x_2 + x_3, \sigma_2 = x_1x_2 + x_1x_3 + x_2x_3, \sigma_3 = x_1x_2x_3
Rule 86 $\sim$ B123/S0 $\sim$ $x'_4 = x_4 + \sigma_3 + \sigma_2 + \sigma_1$

Phase Portrait Modulo Aut ("Hexahedron")

Weight of structure $p = \frac{\text{basin size}}{\text{number of states}}$

Most cycles are spaceships — 36 of 45 or 80%
BW Symmetric Rule 23 $\sim$ B012/S0

$\sim x'_4 = x_4 (\sigma_2 + \sigma_1) + \sigma_3 + 1$

Phase Portrait Modulo $\text{Aut}$ ("Hexahedron")

$p = \frac{9}{32} \approx 0.28$ Limit cycles

$p = \frac{3}{32} \approx 0.09$ Isolated cycles

$p = \frac{33}{128} \approx 0.26$ Limit cycles

$p = \frac{1}{32} \approx 0.03$ Isolated cycles

$p = \frac{3}{16} \approx 0.19$ Isolated cycles

$p = \frac{3}{128} \approx 0.02$ Isolated cycles

$p = \frac{15}{128} \approx 0.12$ Limit cycles

$p = \frac{3}{128} \approx 0.02$ Gardens of Eden

22 spaceships of 61 cycles or about 36%
Quantum Gravity Difficulties:

- Irreversibility of Gravity: information loss (=dissipation) at horizon of black hole
- Reversibility and Unitarity of standard Quantum Mechanics

G. 't Hooft’s approach to reconcile Gravity with Quantum Mechanics:

1. Discrete degrees of freedom at Planck distance scales
2. States of these degrees of freedom form primordial basis of Hilbert space with (nonunitary) evolution
3. Equivalence classes of states: two states are equivalent if they evolve into the same state after some lapse of time
4. Equivalence classes form basis of Hilbert space with unitary evolution governed by time-reversible Schrödinger equation

In our terminology this corresponds to transition to limit cycles: after short time of evolution limit cycles become physically indistinguishable from reversible isolated cycles
Primordial and Unitary Hilbert Spaces

Primordial basis
\[ e_1, e_2, e_3, e_4, e_5, e_6, e_7 \]

Equivalence classes
\[ E_1 = \{ e_1, e_5, e_6, e_7 \} \]
\[ E_2 = \{ e_2 \} \]
\[ E_3 = \{ e_3, e_4 \} \]
form unitary basis

Why irreversibility is not visible: time out of cycle \( \approx 10^{-44} \) sec (Planck time),
time on cycle potentially \( \infty \), minimal time fixed in today’s experiments
\( \approx 10^{-18} \) sec \( \approx 10^{26} \) Planck units
Search For Reversibility

Reversibility is a rare property tending to disappear with growth of complexity of lattice.

### Two rules trivially reversible on all lattices
- 85  ~  B0123/S  ~  $x'_4 = x_4 + 1$
- 170 ~  B/S0123  ~  $x'_4 = x_4$

### Tetrahedron, 6 additional reversible rules
- 43  ~  B0/S012  ~  $x'_4 = x_4 (\sigma_2 + \sigma_1) + \sigma_3 + \sigma_2 + \sigma_1 + 1$
- 51  ~  B02/S02  ~  $x'_4 = \sigma_1 + 1$
- 77  ~  B013/S1  ~  $x'_4 = x_4 (\sigma_2 + \sigma_1 + 1) + \sigma_3 + \sigma_2 + 1$
- 178 ~  B2/S023  ~  $x'_4 = x_4 (\sigma_2 + \sigma_1 + 1) + \sigma_3 + \sigma_2$
- 204 ~  B13/S13  ~  $x'_4 = \sigma_1$
- 212 ~  B123/S3  ~  $x'_4 = x_4 (\sigma_2 + \sigma_1) + \sigma_3 + \sigma_2 + \sigma_1$

### Cube, 2 additional reversible rules
- 51  ~  B02/S02  ~  $x'_4 = \sigma_1 + 1$
- 204 ~  B13/S13  ~  $x'_4 = \sigma_1$

### Dodecahedron and Graphene 6×4, no additional reversible rules
Mesoscopic Lattice Models

- **Non-deterministic** dynamical system — transition from a state to any other state is possible with some probability
- **Markov chain** is typical example
- **Lattice models** are special instances of Markov chains
- **Stationary distributions** of these Markov chains is subject of statistical mechanics
- **Mesoscopic systems** — too large for detailed microscopic description but too small for classical thermodynamics
- **Mesoscopy** studies nuclei, atomic clusters, nanotechnological structures, multi-star systems etc.
Gibbs canonical ensemble with canonical partition function

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

— main tool of conventional statistical mechanics — being essentially asymptotic concept based on “thermodynamic limit” approximation cannot be applied to mesoscopic systems

Instead more fundamental microcanonical ensemble

with entropy formula

\[ S_E = k_B \ln \Omega_E \]

or, equivalently, with microcanonical partition function

\[ \Omega_E = e^{S_E / k_B} \]
Symmetry Approach To Mesoscopic Lattice Models is based on exact enumeration of group orbits of microstates

### Advantages
- Statistical studies are based on simplifying assumptions, it is important to control these assumptions by exact computation, wherever possible.
- Exact computation might reveal subtle details in behavior of systems.

### Example: Ising model
- Vertex values: $s_i \in Q = \{-1, 1\}$
- Hamiltonian: $H = -J \sum_{(i,j)} s_is_j - B \sum_i s_i$
Microcanonical Partition Function

Ising Model On Dodecahedron

Figure: Density of states $\rho(e) = \frac{\Omega_E}{\Omega}$ vs. energy per vertex $e = \frac{E}{|V(\Gamma)|}$
Figure: Specific magnetization \( m(e) = \frac{M(E)}{|V(\Gamma)|} \) vs. energy per vertex \( e \)
In standard thermodynamics

\[ \left. \frac{\partial^2 S}{\partial E^2} \right|_V = -\frac{1}{T^2} \frac{1}{C_V} \implies \text{entropy vs. energy diagramm always concave} \]

\( C_V \) is specific heat

In microcanonical thermodynamics

(mesoscopic and nonextensive systems) there are energy intervals called “convex intruders” where

\[ \left. \frac{\partial^2 S}{\partial E^2} \right|_V > 0 \]

Convex intruders are indicators of first-order phase transitions

Convex intruders in discrete case can be found via easily computed inequality

\[ \Omega^{p+q}_{E_i} < \Omega^p_{E_{i-1}} \Omega^q_{E_{i+1}} \]

where \( p/q = (E_{i+1} - E_i) / (E_i - E_{i-1}) \)
Figure: Microcanonical entropy $s(e) = \ln(\Omega_E) / |V(\Gamma)|$ vs. energy $e$. Left diagram contains distinct convex intruder in interval $-1.2 \leq e \leq -0.9$ and subtle one in interval $-0.8 \leq e \leq -0.6$. Right diagram is fully concave: 1D Ising model has no phase transitions.
Convex Intruders. 3-, 4- and 6-valent Lattices

Figure: Entropy on 3-valent (dot), 4-valent (dash) and 6-valent (solid) tori
Main Results

- **C program** for symmetry analysis of finite discrete dynamical systems has been created
- **Trajectories** of dynamical systems with non-trivial symmetry go always in the direction of **non-increasing** sizes of group **orbits**. Cyclic trajectories lie within orbits of the same size
- **Evolution operators** can be replaced by group shifts after some lapse of time. Initial data tend to form **soliton-like structures**
- **Reversibility** is rare property. Reversible systems are trivial
- **Lattice symmetries** facilitate study (in particular, search of **phase transitions**) of physical **lattice models**