Symmetries and Dynamics of Discrete Systems Talk at CASC 2007, Bonn, Germany

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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

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Discrete Relations and Discrete Dynamical Systems

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)

Lattices and Their Symmetries

- Space of discrete dynamical system is lattice $\Gamma \equiv k$ -valent graph
- Symmetry of lattice Γ is graph automorphism group Aut (Γ)
- We assume Aut (Γ) acts transitively on vertices V(Γ) 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

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Functions on Lattices and Their Orbits

- $Q = \{0, \dots, q-1\}$ is set of values of lattice vertices
- $\Sigma = Q^{\Gamma}$ is space of *Q*-valued functions on Γ
- Aut (Γ) acts non-transitively on Σ splitting this space into orbits of different sizes $\Sigma = \bigcup_{i=1}^{N_{orbits}} O_i$
 - Action: $(g\varphi)(x) = \varphi(g^{-1}x)$ $x \in V(\Gamma), \ \varphi(x) \in \Sigma, \ g \in \operatorname{Aut}(\Gamma)$
- Burnside's lemma counts total number of orbits

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

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

Examples of Lattices



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Cube Is "Smallest Graphene" (Graphene 4×2)

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	<i>V</i> (Г)	Aut(Γ)	$\Omega = q^{ V(\Gamma) }$	Norbits
Tetrahedron	4	24	16	5
Hexahedron	8	48	256	22
Icosahedron	12	120	4096	82
Dodecahedron	20	120	1048576	9436
Graphene 6×4	24	18	16777216	355353
Torus	24	40	10///210	000000
Graphene 6×4	24	16	16777216	1054756
Klein bottle	27	10	10///210	1034730
Triangular 4×6	24	96	16777216	180070
Square 5×5	25	200	33554432	172112
Buckyball	60	120	1152921504606846976	9607679885269312
			$\approx 10^{18}$	pprox 10 ¹⁶

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

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C Program

Input

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

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C Program

Program produces

- automorphism group Aut (Γ)
- Cellular automata branch:
 - phase portraits of automata modulo Aut(Γ) 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

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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"



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

$$\varphi_t(x) = A_t(\varphi(x)) = \varphi\left(g_t^{-1}x\right)$$

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 $\Gamma_{N \times N}$



has the same group $G_{N \times N}$ in both 4-valent

von Neumann \rightarrow and 8-valent Moore \rightarrow cases

Principal case $N = 3, 5, 6, ..., \infty$ $|G_{N \times N}| = 8N^2$ \mathbb{T}^2 is normal $G_{N \times N} = \mathbb{T}^2 \rtimes \mathbb{D}_4$ — semidirect product of \mathbb{T}^2 and \mathbb{D}_4 $\mathbb{T}^2 = \mathbb{Z}_N \times \mathbb{Z}_N$ — translation group $(\mathbb{Z}_\infty \equiv \mathbb{Z})$ $\mathbb{D}_4 = \mathbb{Z}_4 \rtimes \mathbb{Z}_2$ — dihedral group $(\mathbb{Z}_4 - 90^0 \text{ rotations}, \mathbb{Z}_2 - \text{reflections})$ Resembles Euclidean group $\mathbb{E}_2 = (\mathbb{T}^2 = \mathbb{R} \times \mathbb{R}) \rtimes \mathbb{O}(2)$



Group Interpretation of "Glider"

Evolution operator = group action: $\varphi_{t_b}(x) = A_{t_a t_b} (\varphi_{t_a}(x)) = \varphi_{t_a} \left(g_{t_a t_b}^{-1} x \right)$ One step diagonal shift $g_{15} \in \mathbf{T}^2$



One step downward shift \rightarrow 90° clockwise rotation \rightarrow reflection in respect to vertical



Two Examples of Trivalent Cellular Automata with Symmetric Local Rules

• Rule 86 =
$$\overrightarrow{01101010}$$
 ~ $\overrightarrow{B123/S0}$ ~ $\overrightarrow{x_4' = x_4 + \sigma_3 + \sigma_2 + \sigma_1}$

• Rule 23 = 11101000 ~ B012/S0 ~ $x'_4 = x_4 (\sigma_2 + \sigma_1) + \sigma_3 + 1$ 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 ~ B123/S0 ~ $X'_4 = X_4 + \sigma_3 + \sigma_2 + \sigma_1$ 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 Aut ("Hexahedron")



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:
 - Discrete degrees of freedom at Planck distance scales
 - States of these degrees of freedom form primordial basis of Hilbert space with (nonunitary) evolution
 - Equivalence classes of states: two states are equivalent if they evolve into the same state after some lapse of time
 - 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

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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 ∞ , minimal time fixed in today's experiments $\approx 10^{-18}$ sec $\approx 10^{26}$ Planck units

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Search For Reversibility

Reversibility is 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 ~ $x_4^4 = x_4$

Tetrahedron, 6 additional reversible rules

• 43 ~ B0/S012 ~
$$x'_4 = x_4 (\sigma_2 + \sigma_1) + \sigma_3 + \sigma_2 + \sigma_1 + 1$$

• 51
$$\sim$$
 B02/S02 \sim $x_4' = \sigma_1 + 1$

• 77 ~ B013/S1 ~
$$x'_4 = x_4 (\sigma_2 + \sigma_1 + 1) + \sigma_3 + \sigma_2 + 1$$

• 178 ~ B2/S023 ~
$$x'_4 = x_4 (\sigma_2 + \sigma_1 + 1) + \sigma_3 + \sigma_2$$

$$\bullet$$
 204 \sim B13/S13 \sim $x_4^\prime=\sigma_1$

• 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

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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.

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Canonical and Microcanonical Ensembles

Gibbs canonical ensemble with canonical partition function

$$Z = \sum_{\sigma \in \Sigma} \mathrm{e}^{-E_{\sigma}/k_{B}T}$$

 main tool of conventional statistical mechanics — being essentially asymptotic concept based on "thermodynamic limit" approximation can not 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: $H = -J \sum_{(i,j)} s_i s_j B \sum_i s_i$

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Microcanonical Partition Function

Ising Model On Dodecahedron



Magnetization

Ising Model On Dodecahedron



Figure: Specific magnetization $m(e) = M(E) / |V(\Gamma)|$ vs. energy per vertex e

Phase Transitions In Mesoscopic Systems "Convex Intruders"

In standard thermodynamics

 $\frac{\partial^2 S}{\partial E^2}\Big|_V = -\frac{1}{T^2} \frac{1}{C_V} \Longrightarrow \text{ entropy vs. energy diagramm always concave} \\ C_V \text{ is specific heat}$

In microcanonical thermodynamics (mesoscopic and nonextensive systems) there are energy intervals called "convex intruders" where $\frac{\partial^2 S}{\partial E^2}\Big|_V > 0$ Convex intruders are indicators of first-order phase transitions

Convex intruders in discrete case can be found via easily computed inequality $\Omega_{E_i}^{p+q} < \Omega_{E_{i-1}}^{p} \Omega_{E_{i+1}}^{q}$ where $p/q = (E_{i+1} - E_i) / (E_i - E_{i-1})$

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Convex Intruders In Ising Model On Dodecahedron



Figure: Microcanonical entropy $s(e) = \ln (\Omega_E) / |V(\Gamma)|$ vs. energy *e*. Left diagram contains distinct convex intruder in interval $-1.2 \le e \le -0.9$ and subtle one in interval $-0.8 \le e \le -0.6$. 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 traectories 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

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