Symmetry Analysis and Quantization in Discrete Dynamical Systems

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Introduction

Discrete systems are widespread in applications. In particular, many nanostructures are symmetric discrete formations. From a fundamental point of view, there are many philosophical and physical arguments that discreteness is more suitable for describing physics at small distances than continuity which arises only as approximation or as a logical limit in considering large collections of discrete structures. We consider here deterministic and non-deterministic dynamical systems with non-trivial symmetries defined on discrete spaces and evolving in discrete time. As a tool for our study we are developing programs in C based on computer algebra and computational group theory methods.

Basic constituents of discrete models

The following constructions form the basis for all types of dynamical systems under study:

1. *Space* X is a k-valent graph with symmetry group $G = \mathrm{Aut}(X)$ — *space symmetries*.
2. Vertices x of X take values in a set Σ with symmetry group $\Gamma \leq \mathrm{Sym}(\Sigma)$ — *internal symmetries*.
3. *States of the whole system* are functions $\sigma(x) \in \Sigma^X$.
4. We define *whole system symmetry* groups W — unifying space G and internal Γ symmetries — as equivalence classes of *split group extensions* of the form
$$1 \to \Gamma^X \to W \to G \to 1 \ . \qquad (1)$$
5. Action of the group W splits the set of states Σ^X into *orbits* of different sizes:
$$\Sigma^X = \bigsqcup_i O_i \ .$$
6. Evolution proceeds in *discrete time* $t \in \mathbb{Z} = \{\ldots, -1, 0, 1, \ldots\}$.
7. *Dynamics* is determined by some *evolution rule* connecting the current state $\sigma_t(x)$ of the system with its prehistory $\sigma_{t-1}(x)$, $\sigma_{t-2}(x)$, $\sigma_{t-3}(x), \ldots$

For models with locally defined evolution rules — such as, e.g., cellular automata or Ising model — the group of *local symmetries* G_{loc} is essential. G_{loc} is defined as a *stabilizer* of x in G: $G_{loc} = \mathrm{Stab}_G(x)$.

Local rules are defined on *orbits* of G_{loc} on *edges* from the *neighborhoods* of points x. Fig. 1 shows the symmetry groups G and $G_{loc} \leq G$ for some carbon and hydrocarbon molecules.

Let us give an explicit description of the whole symmetry group W. Equivalence classes in (1) are determined by arbitrary *antihomomorphisms* $\mu : G \to G$. The equivalence is described by *arbitrary function* $\kappa : G \to G$. Note that the standard *direct* $\Gamma^X \times G$ and *wreath* $\Gamma \wr_X G$ products are obtained from this general construction by choosing $\mu(a) = 1$ and $\mu(a) = a^{-1}$, respectively. As to the arbitrary function κ, the choices $\kappa(a) = 1$ and $\kappa(a) = a^{-1}$, respectively, are generally used in the literature.

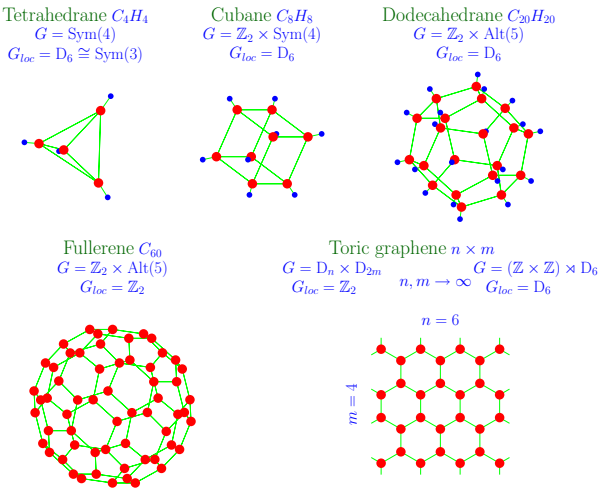


Figure 1: Symmetries of 3-valent (hydro)carbon nanostructures

Deterministic and non-deterministic dynamics

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

$$\sigma_t(x) = F(\sigma_{t-1}(x), \sigma_{t-2}(x), \sigma_{t-3}(x), \ldots) \ . \qquad (2)$$

Cellular automaton is a typical example of the deterministic dynamical system. The causality imposes several restrictions on the system dynamics [1]. In particular, for the first orderfunctional relations:

- *dynamical trajectories* pass group orbits in *non-decreasing* order of orbit sizes,

- *periodic* trajectories lie within orbits of the *same size*.

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

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

Soliton-like structures in deterministic dynamics

For deterministic dynamics recurrence of dynamical trajectory to the same group orbit is typical. Moreover, if the symmetry group W splits the state set Σ^X into a *finite* number of orbits (this is the case for all systems we consider here), 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

$$\sigma_{t_0}(x) \to \sigma_{t_1}(x) = A_{t_1 t_0}\left(\sigma_{t_0}(x)\right) \quad . \qquad (3)$$

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 (3) can be replaced by the *group action*

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

i.e., the initial state $\sigma_{t_0}(x)$ is reproduced after some "*movement*" in the space Σ^X.

Several examples (including continuous cases) of cycles over group orbits:

- *running waves* $\sigma(x - vt)$ in mathematical physics — Galilei group;
- "*generalized coherent states*" in quantum physics — unitary representations of Lie groups;
- "*spaceships*" in cellular automata — lattice symmetries.

Fig. 2 illustrates formation of "glider" — one of the "spaceships" in Conway's cellular automaton "Game of Life".

Mesoscopic lattice models

Discrete symmetry analysis simplifies manipulations with *microcanonical ensembles* and search of *phase transitions*. This allows one to reveal subtle details in behavior of *mesoscopic models*: in Fig. 3 in addition to distinct "*convex intruder*" — criterion of phase transition adopted in *mesoscopy* — denoted A computation detects subtle "intruder" B.

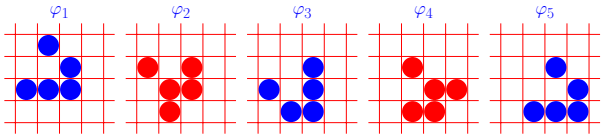


Figure 2: Example of a soliton-like structure. "Glider" in Conway's "Life"is a cycle in *two* orbits of the square lattice symmetry group (semidirect product of 2D translations and dihedral group D_8): configurations φ_3 and φ_4 are obtained from φ_1 and φ_2, respectively, by *the same* combination of downward *shift*, 90^o clockwise *rotation* and *reflection* in respect to vertical

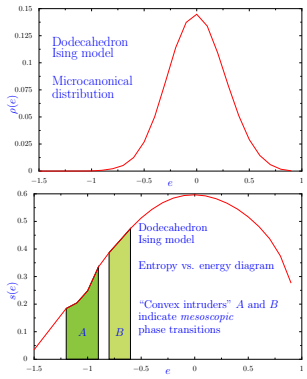


Figure 3: Ising model on dodecahedron. Microcanonical distribution and "convex intruders" indicating *mesoscopic* phase transitions

Gauge connection and quantization

The Aharonov–Bohm effect (Fig. 4) is one of the most striking 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 decomposes into the product of elements of the fundamental representation of the group $\Gamma = \mathrm{U}(1)$:

$$A_{\mathrm{U}(1)} = \exp\left(iS\right) = \exp\left(i\int L dt\right)$$

$$\longrightarrow \quad \mathrm{e}^{iL_{0,1}} \ldots \mathrm{e}^{iL_{t-1,t}} \ldots \mathrm{e}^{iL_{T-1,T}} . \qquad (4)$$

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

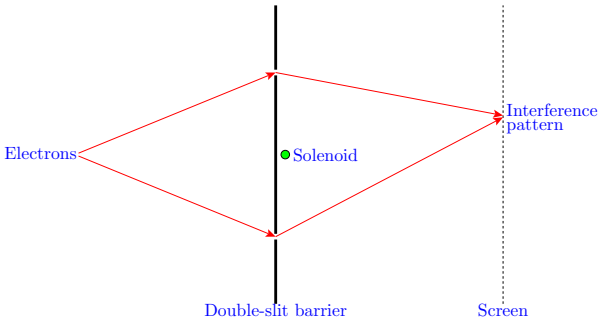


Figure 4: Aharonov–Bohm effect. Magnetic flux is confined within the perfectly shielded solenoid; interference pattern is shifted in spite of absence of electromagnetic forces acting on the particles

physics where the typical Lagrangians are depend on the *first order* derivatives. Thus, the expression $P(t-1,t) = e^{iL_{t-1,t}} \in \mathrm{U}(1)$ can be interpreted as U(1)-parallel transport. A natural generalization of this is to suppose that:

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

We can introduce a quantum mechanical description of a discrete system interpreting states $\sigma \in \Sigma$ as basis elements of a Hilbert space Ψ. This allows one to describe statistics of observations of σ's in terms of the *inner product* in Ψ.

Now let us replace expression (4) for Feynman's path amplitude by the following parallel transport along the path

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

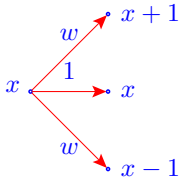
Here $\alpha_{t-1,t}$ are elements of a *finite group* Γ — we shall call Γ *quantizing group* — and ρ is an unitary representation of Γ on the space Ψ.

Recall that all linear representations of finite groups are (equivalent to) unitary and all their *characters* and *eigenvalues* are elements of the ring $\mathbb{A}$ of *algebraic integers*. It is not difficult to show [2] that algebraic integers are sufficient for all our computations (except for normalization of probabilities requiring the *quotient field* of the ring $\mathbb{A}$). Thus, with our approach the quantization becomes a completely *constructive* procedure. On the other hand, the standard Feynman's quantization can be approximated within our approach by taking 1-dimensional representations of large enough finite groups.

Simple model inspired by free particle

In quantum mechanics — as is clear from the *never vanishing* expression $\exp\left(\frac{i}{\hbar}S\right)$ for the path amplitude — transitions from one to any other state are possible in principle. However 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 $L = \frac{m\dot{x}^2}{2}$. Keeping only transitions to the closest points in the discretized space we come to the following rule for the one-time-step transition amplitudes



$$e^{\frac{i}{\hbar}\frac{m\{(x+1)-x\}^2}{2}} = e^{i\frac{m}{2\hbar}}$$

$$e^{\frac{i}{\hbar}\frac{m(x-x)^2}{2}} = 1$$

$$e^{\frac{i}{\hbar}\frac{m\{(x-1)-x\}^2}{2}} = e^{i\frac{m}{2\hbar}}.$$

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

$$R(x \to x) = 1 \quad \in \quad \mathrm{U}(1),$$

$$R(x \to x-1) = R(x \to x+1)$$

$$= w = e^{i\frac{m}{2\hbar}} \quad \in \quad \mathrm{U}(1). \quad (5)$$

Now let us assume that w in (5) is an element of some representation of a finite group: $w = \rho(\alpha)$, $\alpha \in \Gamma = \{\gamma_0 = 1, \dots, \gamma_{M-1}\}$. Rearranging *multinomial coefficients* — *trinomial* in this concrete case — it is not difficult to write the sum amplitude over all paths of the form $(0,0) \longrightarrow (x,t)$

$$A_x^t(w) = \sum_{\tau=0}^{t} \frac{\tau!}{\left(\frac{\tau-x}{2}\right)!\left(\frac{\tau+x}{2}\right)!} \times \frac{t!}{\tau!\,(t-\tau)!}\, w^\tau \quad . \quad (6)$$

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 one-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 $\Gamma = \mathbb{Z}_M = \{\gamma_0, \cdots, \gamma_k, \cdots, \gamma_{M-1}\}$. Any of its M irreducible representations takes the form $\rho(\gamma_k) = w^k$, where w is one of the Mth roots of unity. For simplicity let w be the *primitive root*: $w = \mathrm{e}^{2\pi i/M}$.

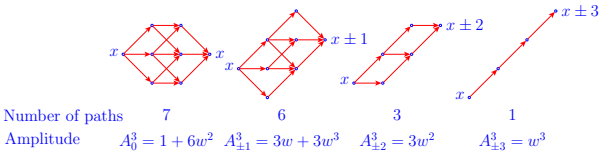


Figure 5: Amplitudes for all possible paths in three time steps

Fig. 5 shows all possible transitions (with their amplitudes) from the point x in three time steps. We see that the polynomial $A^3_{\pm1} = 3w + 3w^3 = 3w\left(w^2 + 1\right)$ 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 $\mathbb{Z}_4$. Thus, $\mathbb{Z}_4$ is the natural quantizing group for the model under consideration.

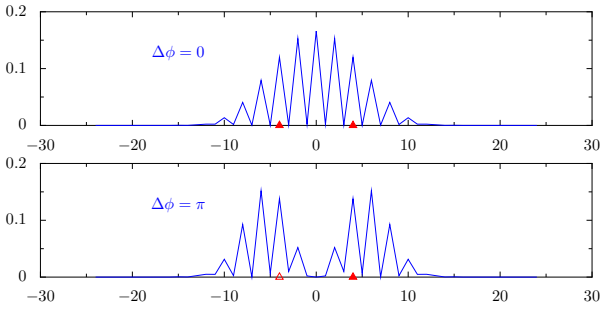


Figure 6: Group $\mathbb{Z}_4$. Interference from two sources at points -4 and 4. Number of time steps $T = 20$. Phase differences $\Delta\phi = \phi_4 - \phi_{-4}$ between sources are 0 and π.

Fig. 6 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 the interference pattern when sources are in the same ($\Delta\phi = 0$) and in the opposite ($\Delta\phi = \pi$) phases, respectively.

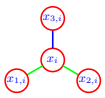
Local quantum models on regular graphs

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

1. *Space* $X = \{x_1, \cdots, x_N\}$ is a $k-$valent graph.
2. *Set of local transitions* $E_i = \{e_{0,i}, e_{1,i}, \cdots, e_{k,i}\}$ 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 $G = \mathrm{Aut}(X)$ acts transitively on the set $\{E_1, \cdots, E_N\}$.
4. $G_i = \mathrm{Stab}_G(x_i) \leq G$ is the *stabilizer* of x_i ($g \in G_i$ means $x_i g = x_i$).
5. $\Omega_i = \{\omega_{0,i}, \omega_{1,i}, \cdots, \omega_{h,i}\}$ is the *set of orbits* of G_i on E_i.
6. *Quantizing group* Γ is a finite group: $\Gamma = \{\gamma_0, \cdots, \gamma_{M-1}\}$.
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 Ω_i, i.e., $R(e_{m,i}g) = R(e_{m,i})$ for $g \in G_i$.

To illustrate these constructions, let us consider the local quantum model on the graph of *buckyball*. The incarnations of this 3-valent graph include in particular:

- the *Caley graph of the icosahedral group* Alt(5) (in mathematics);
- the *molecule* C_{60} (in carbon chemistry).

Here the space $X = \{x_1, \cdots, x_{60}\}$ has the shape  and its symmetry group is $G = \mathrm{Aut}(X) = \mathbb{Z}_2 \times \mathrm{Alt}(5)$. The set of local transitions takes the form $E_i = \{e_{0,i},\ e_{1,i},\ e_{2,i},\ e_{3,i}\}$, where $e_{0,i} = (x_i \to x_i)$, $e_{1,i} = (x_i \to x_{1,i})$, $e_{2,i} = (x_i \to x_{2,i})$, $e_{3,i} = (x_i \to x_{3,i})$ in accordance with 

The stabilizer of x_i is $G_{loc} = \mathrm{Stab}_G(x_i) = \mathbb{Z}_2$. 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 $(x_i \to x_i)$ and

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

The evolution rule takes the form:

$$R(x_i \to x_i) = \rho(\alpha_0),$$
$$R(x_i \to x_{1,i}) = R(x_i \to x_{2,i}) = \rho(\alpha_1),$$
$$R(x_i \to x_{3,i}) = \rho(\alpha_2),$$

where $\alpha_0, \alpha_1, \alpha_2 \in \Gamma$. If we take a one-dimensional representation and move α_0 — using gauge invariance — to the identity element of Γ, 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.

Summary

We suggested an algorithmic approach based on a discrete symmetry analysis and implemented in C for construction and investigation of discrete dynamical models — *deterministic*, *mesoscopic* and *quantum*. In particular, our approach is applicable to simulation of nanostructures with nontrivial symmetry properties. Important examples of such nanostructures are (hydro)carbon molecules like graphenes, fullerenes, etc.

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

We demonstrated that soliton-like moving structures — like "*spaceships*" in cellular automata — arise inevitably in *deterministic* dynamical systems whose symmetry group splits the set of states into finite number of group orbits.

We proposed a method based on introduction of gauge connection of a special kind for quantizing discrete systems and constructed simple models for studying properties of suggested quantization.

We hope that the discrete and finite background allowing a comprehensive study may lead to a deeper understanding of the quantum behavior and its connection with symmetries, especially with gauge symmetries, of systems. To study more complicated models, we are developing C programs based on computer algebra and computational group theory methods.

References

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