SYMMETRIES, GAUGE INVARIANCE AND QUANTIZATION IN DISCRETE MODELS[1]

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Different aspects of discrete symmetry analysis in application to deterministic and non-deterministic lattice models are considered. One of the main tools for our study are programs written in C. In the case of deterministic dynamical systems, such as cellular automata, the non-trivial connections between the lattice symmetries and dynamics are discussed. In particular, we show that the formation of moving soliton-like structures — analogs of "spaceships" in cellular automata or "generalized coherent states" in quantum physics — results from the existence of a non-trivial symmetry group. In the case of mesoscopic lattice models, we apply some algorithms exploiting the symmetries of the models to compute microcanonical partition functions and to search phase transitions. We also consider the gauge invariance in discrete dynamical systems and its connection with quantization. We propose a constructive approach to introduce quantum structures in discrete systems based on finite gauge groups. In this approach, quantization can be interpreted as the introduction of a gauge connection of a special kind. We illustrate our approach to quantization by a simple model and propose its generalization.

Keywords: symmetries of discrete systems, gauge principle, quantization.

1. Introduction. Discrete systems are widespread in applications. In particular, many nanostructures are symmetric discrete formations (see, e.g., Fig. 1).
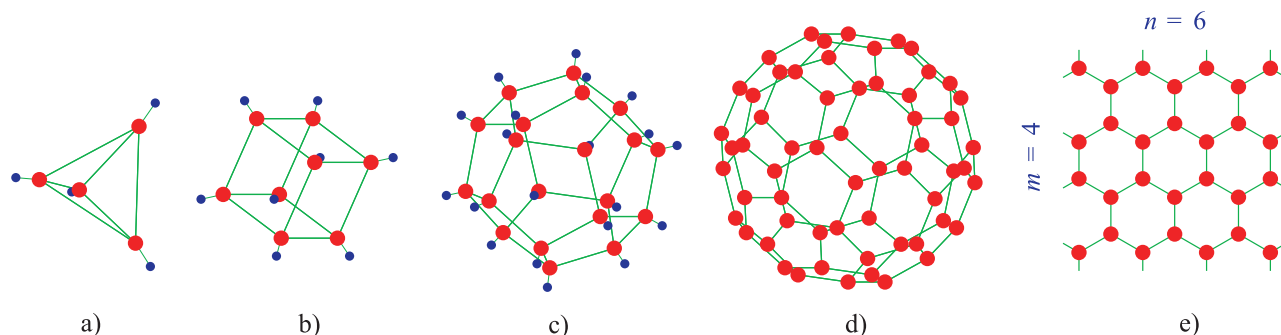

Fig. 1. Symmetries of 3-valent (hydro)carbon nanostructures:
a) Tetrahedrane C_4H_4 ($G = \mathrm{Sym}(4)$, $G_{\mathrm{loc}} = D_6 \cong \mathrm{Sym}(3)$); b) Cubane C_8H_8 ($G = \mathbb{Z}_2 \times \mathrm{Sym}(4)$, $G_{\mathrm{loc}} = D_6$;
c) Dodecahedrane $C_{20}H_{20}$ ($G = \mathbb{Z}_2 \times \mathrm{Alt}(5)$, $G_{\mathrm{loc}} = D_6$; d) Fullerene C_{60} ($G = \mathbb{Z}_2 \times \mathrm{Alt}(5)$, $G_{\mathrm{loc}} = \mathbb{Z}_2$;
e) Toric graphene $n \times m$ ($G = D_n \times D_{2n}$, $G_{\mathrm{loc}} = \mathbb{Z}_2$; n, $m \to \infty$, $G = (\mathbb{Z} \times \mathbb{Z}) \rtimes D_6$, $G_{\mathrm{loc}} = D_6$

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 the continuity that arises only as an approximation or as a logical limit in considering large collections of discrete structures. In 1912 Henri Poincaré wrote [1]: "We now wonder not only whether the differential equations of dynamics must be modified, but whether the laws of motion can still be expressed by means of differential equations ... . It is being asked whether it is not necessary to introduce discontinuities into the natural laws, not apparent ones but essential ones". Since that time, the number and weights of arguments supporting similar views have increased considerably.

In this paper we consider 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 [2].

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2. Basic constituents of discrete models. In this paper we consider the following constructions that form a basis for all types of dynamical systems:

1) a space X is a k-valent graph with the symmetry group $G = \mathrm{Aut}(X)$ — *space symmetries*;

2) the vertices x of X take values in a set Σ with the symmetry group $\Gamma \leqslant \mathrm{Sym}(\Sigma)$ — *internal symmetries*;

3) *the states of the whole system* are functions $\sigma(x) \in \Sigma^X$;

4) we define *the whole system symmetry* groups W — unifying the space G and the internal Γ symmetries — as the equivalence classes of *split group extensions* [3] of the form

$$1 \to \Gamma^X \to W \to G \to 1 \,; \tag{1}$$

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* $t \in \mathbb{Z} = \{\dots, -1, 0, 1, \dots\}$;

7) *dynamics* is determined by some *evolution rule* connecting the current state $\sigma_t(x)$ of the system with its prehistory $\sigma_{t-1}(x)$, $\sigma_{t-2}(x)$, $\sigma_{t-3}(x)$, $\dots$.

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 and is defined as a *stabilizer* of a vertex x in the space group G: $g \in G_{\mathrm{loc}} = \mathrm{Stab}_G(x)$ means $xg = x$. Local rules are defined on *orbits* of G_{loc} on *edges* from the *neighborhoods* of the points x. Figure 1 shows the symmetry groups G and $G_{\mathrm{loc}} \leqslant G$ for some carbon and hydrocarbon molecules.

Let us give an explicit description of the whole symmetry group W. The equivalence classes in (1) are determined by arbitrary *antihomomorphisms* $\mu : G \to G$. The term "antihomomorphism" means that $\mu(a)\mu(b) = \mu(ba)$. The equivalence is described by *arbitrary function* $\kappa : G \to G$. The explicit formulas for the main group operations — *action*[3] on Σ^X, *multiplication*, and *inversion* — are

$$
\begin{aligned}
\sigma(x)\big(\alpha(x), a\big) \quad &= \sigma\big(x\mu(a)\big)\,\alpha\big(x\kappa(a)\big)\,, \\
\big(\alpha(x), a\big)\big(\beta(x), b\big) &= \Big(\big(\alpha\big(x\kappa(ab)^{-1}\mu(b)\kappa(a)\big)\beta\big(x\kappa(ab)^{-1}\kappa(b)\big)\big), ab\Big)\,, \\
\big(\alpha(x), a\big)^{-1} \quad &= \Big(\alpha\big(x\kappa(a^{-1})^{-1}\mu(a)^{-1}\kappa(a)\big)^{-1}, a^{-1}\Big)\,.
\end{aligned}
$$

Here $\big(\alpha(x), a\big) \in W$ with $\alpha(x) \in \Gamma^X$ and $a \in G$, etc. Note that the standard *direct* and *wreath* 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. Thus, the action and multiplication take the following forms for the *direct product* $\Gamma^X \times G$: $\sigma(x)\big(\alpha(x), a\big) = \sigma(x)\alpha(x)$, $\big(\alpha(x), a\big)\big(\beta(x), b\big) = \big(\alpha(x)\beta(x), ab\big)$ and for the *wreath product* $\Gamma \wr_X G$: $\sigma(x)\big(\alpha(x), a\big) = \sigma(xa^{-1})\alpha(xa^{-1})$, $\big(\alpha(x), a\big)\big(\beta(x), b\big) = \big(\alpha(x)\beta(xa), ab\big)$.

3. Deterministic and non-deterministic dynamics. The 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:

$$\sigma_t(x) = F\big(\sigma_{t-1}(x), \sigma_{t-2}(x), \sigma_{t-3}(x), \dots\big)\,. \tag{2}$$

Cellular automaton is a typical example of a deterministic dynamical system. The causality imposes severe restrictions on the system dynamics [4]. In particular, for the first-order[4] functional relations:

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

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

A *mesoscopic lattice model* is a type of non-deterministic dynamical systems. This is a special case of a *Markov chain*. In a mesoscopic lattice model, the transition from one state to any other is possible with a probability controlled by a Hamiltonian.

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

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

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[3]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]This means that (2) takes the form $\sigma_t(x) = F\big(\sigma_{t-1}(x)\big)$.

any trajectory comes *inevitably* to a cycle over some finite sequence of orbits. This just means the formation of *soliton-like structures*. Namely, let us consider the evolution

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

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

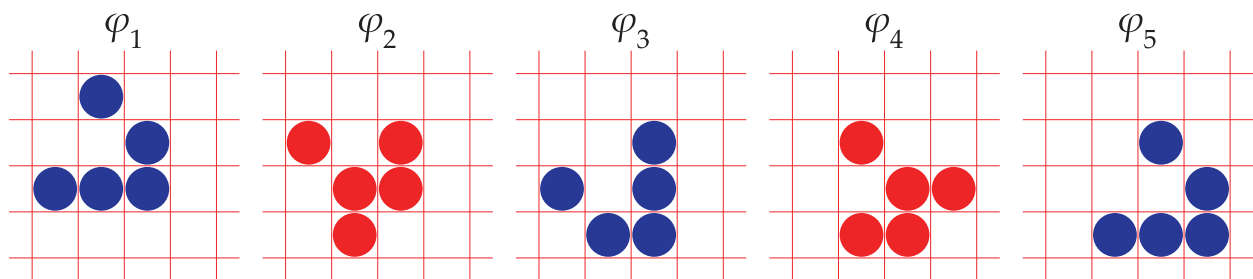— "*spaceships*" in cellular automata — lattice symmetries.

Fig. 2. Example of soliton-like structure

Figure 2 illustrates the formation of "glider" — one of the "spaceships" in Conway's cellular automaton "Game of Life". "Glider" in Conway's "Life" is a cycle in *two* orbits of the square lattice symmetry group (the semidirect product of 2D translations and dihedral group D_8): the configurations φ_3 and φ_4 are obtained from φ_1 and φ_2, respectively, by *the same* combination of downward *shift*, 90° clockwise *rotation* and *reflection* with respect to the vertical.
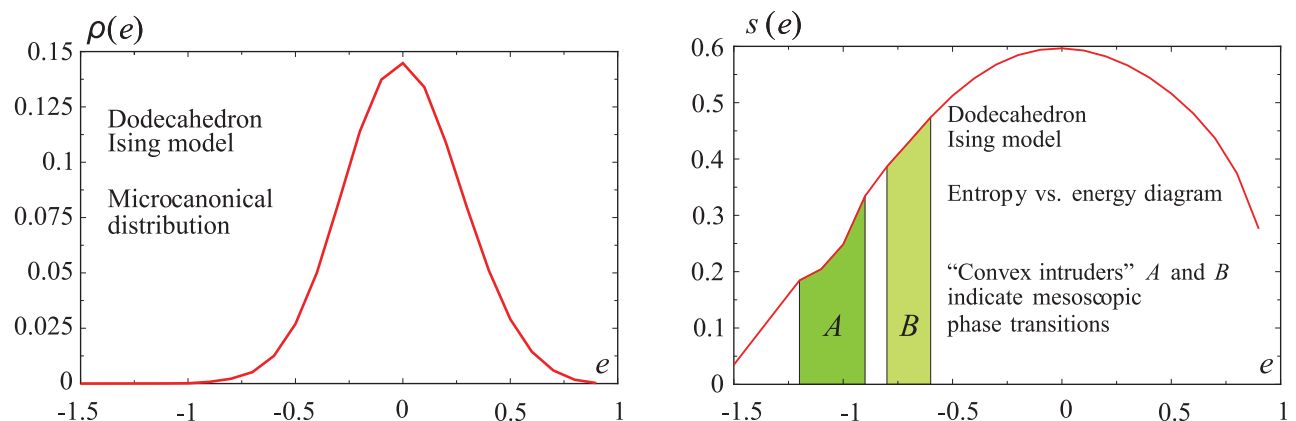

Fig. 3. Ising model on dodecahedron. Microcanonical distribution and "convex intruders" indicating *mesoscopic* phase transitions

5. Mesoscopic lattice models. The discrete symmetry analysis simplifies the manipulations with *microcanonical ensembles* and the search of *phase transitions*. This allows one to reveal subtle details in the behavior of *mesoscopic models*: in addition to distinct "*convex intruder*" denoted by A (a criterion of phase transition adopted in *mesoscopy*), in Fig. 3 we see that the computation detects a subtle "intruder" B.

6. Discrete gauge principle. In fact, the gauge principle expresses the general idea that any observable data can be presented in different "frames" at different points and there should be some way to compare these data. At the set-theoretic level suitable for both the discrete and the continuous cases, the main concepts of the gauge principle can be reduced to the following elements:

— a set X, space or space-time;

— a set Σ, local states;

— the set Σ^X of Σ-valued functions on X, the set of states of *dynamical systems*;

— a group $W \leqslant \mathrm{Sym}(\Sigma^X)$ acting transitively on Σ^X, *symmetries of the system*;

— identification of data describing a dynamical system makes sense only *modulo* symmetries from W;

— having no *a priori* connection between data from Σ^X at different points x and y in time and space, we impose this *connection* (or *parallel transport* [5]) explicitly as W-valued functions on edges of an *abstract* graph: $P(x,y) \in W$, $\varsigma(y) = \sigma(x)P(x,y)$; the connection $P(x,y)$ has the obvious property $P(y,x) = P(x,y)^{-1}$;

— a connection $\widetilde{P}(x,y)$ is called *trivial* if it can be expressed in terms of a function on the *vertices* of a graph: $\widetilde{P}(x,y) = r(x)^{-1}r(y)$, $r(x)$, $r(y) \in W$;

— invariance with respect to gauge symmetries depending on time or space $u(x) \in W$, $u(y) \in W$ leads to the transformation rule for connection: $P(x,y) \to u(x)^{-1}P(x,y)u(y)$;

— the *curvature* of a connection $P(x,y)$ is defined as the conjugacy class of the *holonomy* along a cycle of a graph: $P(x_1, x_2, \ldots, x_k) = P(x_1, x_2)P(x_2, x_3)\ldots P(x_k, x_1)$ (the conjugacy means that $P'(x_1, \ldots, x_k) \sim u^{-1}P(x_1, \ldots, x_k)u$ for any $u \in W$); the curvature of trivial connection is obviously trivial: $\widetilde{P}(x_1, \ldots, x_k) \equiv 1$;

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

Standard continuous gauge theories can easily be deduced from the above description by expansion of the parallel transport $P(x,y)$ for two closely situated points x and $x + \Delta x$ in continuous space with taking into account that $P(x,x) = 1$. This leads to the introduction of a Lie algebra valued 1-form A: $P(x, x + \Delta x) \approx 1 + A\Delta x$. The curvature 2-form $F = dA + [A \wedge A]$ is interpreted as a *physical strength field*. Finally, one should write dynamical equations for the gauge fields. The most important example of gauge dynamics is the *Yang–Mills theory* with the equations of motion
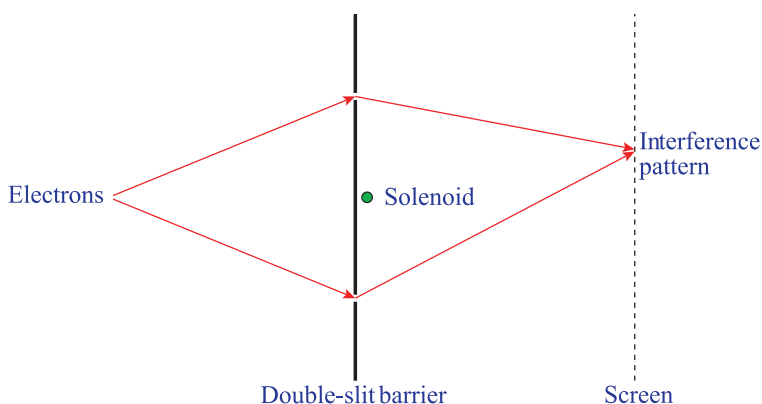

Fig. 4. Aharonov–Bohm effect. Magnetic flux is confined within the perfectly shielded solenoid; interference pattern is shifted in spite of absence of electromagnetic forces acting on the particles

$$\mathrm{d}F + [A \wedge F] = 0\,, \tag{4}$$
$$\mathrm{d} \star F + [A \wedge \star F] = 0\,.$$

Note that (4) is *a priori* (empty) statement called the *Bianci identity*. Note also that the Yang–Mills equations for the Abelian gauge group $\mathrm{U}(1)$ are the same as Maxwell's equations.

7. 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 a 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 the working solenoid produces the $\mathrm{U}(1)$-connection, adding or subtracting the phases of the particles and thus changing the interference pattern.

In the discrete time, Feynman's path amplitude [6] is decomposed into the product of elements of the fundamental representation of the group $\Gamma = \mathrm{U}(1)$:

$$A_{\mathrm{U}(1)} = \exp(iS) = \exp\left(i \int L\,dt\right) \longrightarrow e^{iL_{0,1}} \ldots e^{iL_{t-1,t}} \ldots e^{iL_{T-1,T}}\,. \tag{5}$$

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 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 the $\mathrm{U}(1)$-parallel transport. A natural generalization of this is to suppose that

— the group Γ may differ from $\mathrm{U}(1)$,

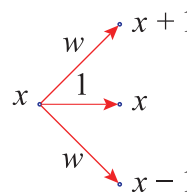— the dimension of the unitary representation $\rho(\Gamma)$ may differ from 1.

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

Now let us replace expression (5) for Feynman's path amplitude by the following parallel transport along the path $A_{\rho(\Gamma)} = \rho(\alpha_{0,1}) \ldots \rho(\alpha_{t-1,t}) \ldots \rho(\alpha_{T-1,T})$. Here $\alpha_{t-1,t}$ are the elements of a *finite group* Γ — we shall call Γ a *quantizing group* — and ρ is a 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*[5] [7]. It is not difficult to show [8] that algebraic integers are sufficient for all our computations (except for normalization of probabilities requiring the *quotient field* of the ring $\mathbb{A}$). With our approach, thus, the quantization becomes a completely *constructive* procedure. On the other hand, the standard Feynman's quantization can be approximated within our approach by taking the 1-dimensional representations of sufficiently large finite groups.

8. A simple model induced by a free particle. In quantum mechanics, as is clear from the *never vanishing* expression $\exp\left(\dfrac{i}{\hbar} S\right)$ for the path amplitude, the transitions from one to any other state are possible in principle. However, we shall consider a 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 $L = m\dot{x}^2/2$. Keeping only the transitions to the closest points in the discretized space, we come to the following rule for the one-time-step transition amplitudes:

$$e^{im\{(x+1)-x\}^2/(2\hbar)} = e^{im/(2\hbar)},$$

$$e^{im(x-x)^2/(2\hbar)} = 1,$$

$$e^{im\{(x-1)-x\}^2/(2\hbar)} = e^{im/(2\hbar)}.$$

In other words, we have the evolution rule as a U(1)-valued function R defined on pairs of points (graph edges). Symbolically:

$$R(x \to x) = 1 \in \mathrm{U}(1),$$
$$R(x \to x-1) = R(x \to x+1) = w = e^{im/(2\hbar)} \in \mathrm{U}(1). \tag{6}$$

Now let us assume that w in (6) is an element of some representation of a finite group: $w = \rho(\alpha)$, $\alpha \in \Gamma = \{\gamma_0 = 1, \ldots, \gamma_{M-1}\}$.

Rearranging *multinomial coefficients* (*trinomial* in this particular case) it is not difficult to write the sum amplitude over all paths of the form $(0,0) \longrightarrow (x,t)$: $A_x^t(w) = \displaystyle\sum_{\tau=0}^{t} \frac{\tau!}{\left(\dfrac{\tau-x}{2}\right)! \left(\dfrac{\tau+x}{2}\right)!} \frac{t!}{\tau!(t-\tau)!} w^\tau$. 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* — the 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 the 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 $w^M = 1$. To be specific, let us consider the cyclic group $\Gamma = \mathbb{Z}_M = \{\gamma_0, \ldots, \gamma_k, \ldots, \gamma_{M-1}\}$. 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*: $w = e^{2\pi i/M}$.

Figure 5 shows all possible transitions (with their amplitudes) from the point x in three time steps. We see that the polynomial $A_{\pm 1}^3 = 3w + 3w^3 = 3w(w^2 + 1)$ 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 shows interference patterns — normalized squared amplitudes ("probabilities") — from two sources placed in the positions $x = -4$ and $x = 4$ for 20 time steps. The left and right graphs show interference pattern when sources are in the same ($\Delta\phi = 0$) and in the opposite ($\Delta\phi = \pi$) phases, respectively.

9. Local quantum models on regular graphs. The above model — with quantum transitions allowed

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[5]The ring $\mathbb{A}$ consists of the roots of *monic* polynomials with integer coefficients [3].

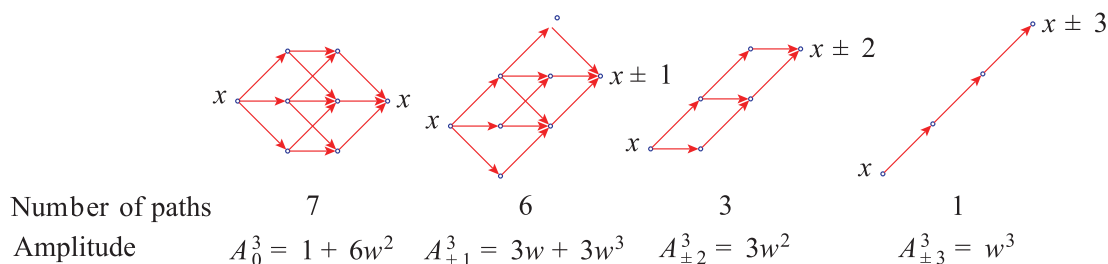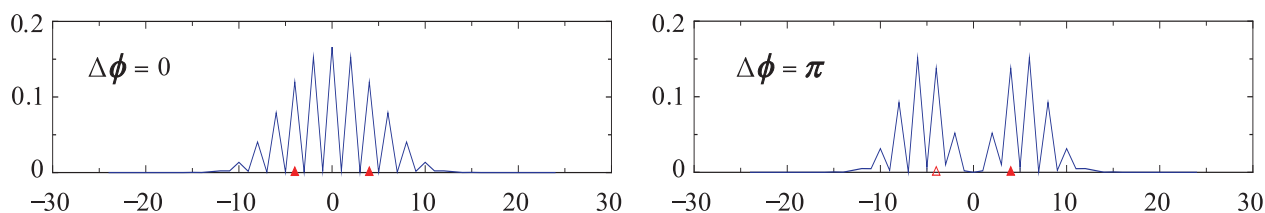| Number of paths	7	6	3	1
Amplitude	$A_0^3 = 1 + 6w^2$	$A_{\pm 1}^3 = 3w + 3w^3$	$A_{\pm 2}^3 = 3w^2$	$A_{\pm 3}^3 = w^3$

Fig. 5. Amplitudes for all possible paths in three time steps

Fig. 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

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

     1. The *space* $X = \{x_1, \ldots, x_N\}$ is a $k-$valent graph.

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

Fig. 7   Fig. 8

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

     4. $G_{\mathrm{loc}} = \mathrm{Stab}_G(x_i) \leqslant G$ is a *stabilizer* of x_i.

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

     6. the *quantizing group* Γ is a finite group: $\Gamma = \{\gamma_0, \ldots, \gamma_{M-1}\}$.

     7. the *evolution rule* R is a function on E_i with its values in some representation $\rho(\Gamma)$. The rule R prescribes $\rho(\Gamma)$-weights to the one-time-step transitions from x_i to the elements of the neighborhood of x_i. From the symmetry considerations, R must be a function on orbits from Ω_i, i.e., $R(e_{mi}g) = R(e_{mi})$ for $g \in G_{\mathrm{loc}}$.

     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* $\mathrm{Alt}(5)$ (in mathematics);

     — the *molecule C_{60}* (in carbon chemistry).

Here the space $X = \{x_1, \ldots, x_{60}\}$ has the shape of Fig. 7 and its symmetry group is $G = \mathrm{Aut}(X) = \mathbb{Z}_2 \times \mathrm{Alt}(5)$. The set of local transitions takes the form $E_i = \{e_{0i}, e_{1i}, e_{2i}, e_{3i}\}$, where $e_{0i} = (x_i \to x_i)$, $e_{1i} = (x_i \to x_{1i})$, $e_{2i} = (x_i \to x_{2i})$, $e_{3i} = (x_i \to x_{3i})$ in accordance with Fig. 8. The stabilizer of x_i is $G_{\mathrm{loc}} = \mathrm{Stab}_G(x_i) = \mathbb{Z}_2$. The set of orbits of G_{loc} on E_i contains the three orbits: $\Omega_i = \{\omega_{0i} = \{e_{0i}\}, \omega_{1i} = \{e_{1i}, e_{2i}\}, \omega_{2i} = \{e_{3i}\}\}$, i.e., the stabilizer does not move the edges $(x_i \to x_i)$ and $(x_i \to x_{3i})$ and swaps $(x_i \to x_{1i})$ and $(x_i \to x_{2i})$. This asymmetry results from the different roles the edges play in the structure of the buckyball: $(x_i \to x_{1i})$ and $(x_i \to x_{2i})$ are edges of a pentagon adjacent to x_i, whereas $(x_i \to x_{3i})$ separates two hexagons; in the carbon molecule C_{60}, the edge $(x_i \to x_{3i})$ corresponds to the double bond, whereas the others are the single bonds.

     The evolution rule takes the form

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

where α_0, α_1, and $\alpha_2 \in \Gamma$. If we take a one-dimensional representation and move α_0 — using the gauge invariance — to the identity element of Γ, we see that the rule R depends on the 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., the Gröbner basis
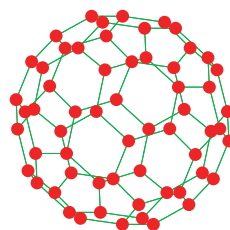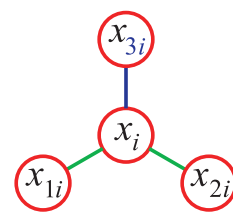
computation) the compatibility of the system of polynomial equations $A(v, w) = \Phi_i(v) = \Phi_j(w) = 0$, where $\Phi_i(v)$ and $\Phi_j(w)$ are cyclotomic polynomials.

10. Summary. We proposed an algorithmic approach based on discrete symmetry analysis and implemented in C for the construction and investigation of discrete dynamical models — *deterministic, mesoscopic,* and *quantum.* In particular, our approach is applicable to the 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 the 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 the *deterministic* dynamical systems whose symmetry group splits the set of states into a finite number of group orbits.

We formulated the gauge principle in the form most suitable for discrete and finite systems. We also proposed a method based on the introduction of gauge connection of a special kind for quantizing discrete systems and constructed simple models for studying the properties of the suggested quantization. We hope that the discrete and finite background allowing comprehensive study may lead to a 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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