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Rotators, Periodicity, and Absence of Diffusion in Cyclic Cellular Automata

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Cyclic cellular automata are two-dimensional cellular automata which generalize lattice versions of the Lorentz gas and certain biochemistry models of artificial life. We show that rotators and time reversibility play a special role in the creation of closed orbits in cyclic cellular automata. We also prove that almost every orbit is closed (periodic) and the absence of diffusion for the flipping rotator model (also known as the ant).

KEY WORDS: Cellular automata; closed orbit; periodic point; rotators; time reversibility; Lorentz lattice gas.

1. INTRODUCTION

The study of the nature of motion of a tagged particle in a fluid has a long history. There are two types of models which were created in these efforts: deterministic ones and probabilistic ones. Deterministic models are more physically relevant to the initial problem of deriving the macroscopic dynamics from the microscopic laws. The first such model is the Boltzmann gas of hard spheres,[1] where one considers the diffusion of a tagged particle in a gas of identical particles. Later models include the Lorentz gas[2] and Ehrenfest's wind-tree model.[3] In these two models a point particle moves in an array of immovable (infinitely heavy) scatterers.

The study of these models turned out to be very complicated. Therefore recently simpler deterministic models were considered. These models form the class of Lorentz lattice gas cellular automata.[4-6] In biochemistry a related class of cellular automata was considered in the description of

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artificial life.[7] These models demonstrate a large variety of different kinds of motion.[8-10] They are deterministic dynamical systems in a random environment.

In this paper we consider a class of models which generalize Lorentz lattice gas cellular automata. In cyclic cellular automata one (or many) point particles propagate with unit speed along the bonds of some lattice. At any vertex the velocity direction of the particle is changed according to a deterministic scattering rule. The scattering rule chosen depends on the state of the vertex. The states of a vertex change cyclically, hence the name cyclic cellular automata. In comparison, in Lorentz lattice gas models there are only one or two states. A cyclic cellular automaton is defined by a lattice (square, triangular, hexagonal, quasicrystal, etc.), by a collection of admissible scattering rules with an ordering (states), and by their distribution among the vertices of the lattice.

In refs. 8–10 we showed that taking different lattices and scattering rules, one gets different behavior of the motion in the corresponding Lorentz lattice gas cellular automata. This is the traditional (direct) approach to the analysis of models in kinetic theory, that is, one defines a model and then analyzes its dynamics, in particular the topology of trajectories of particles.

In this paper we show (for the first time, to our knowledge) that it is possible to consider and to solve in some cases the inverse problem, i.e., the topology of trajectories of a moving particle (the macroscopic dynamics) defines the types of immovable particles (the microscopic scattering laws) and some features of their distribution on a lattice. Moreover, we have found some relations of time reversibility in Lorentz lattice gas cellular automata with the topology of trajectories of the particle.

Our main result is that in the absence of backscattering on the square lattice the existence of a closed (periodic) trajectory (at least one!) of a particle implies that all scattering rules are rotations by $90°$ (rotators). Because rotators are singled out we go on to show that for the flipping rotator model (also known as the ant) almost every orbit is closed and this model exhibits an absence of diffusion.

We have found that time reversibility and the existence of periodic motion are closely linked for cyclic cellular automata. It would be interesting to see what the relation between them is for other classes of such models, for example, FCHC-lattice gas cellular automata.[11]

2. DESCRIPTION OF THE MODELS AND STATEMENT OF THEOREMS

We consider the $\mathbf{Z}^2$ lattice. All (or some) vertices contain an identical copy of the same finite automaton which can be in any one of k states. We think of the finite automaton in a given state as a scattering rule. Namely in $\mathbf{Z}^2$ label the four edges coming to a vertex 0, 1, 2, 3 so that on a clock the edge i corresponds to $3i$ o'clock. A scattering rule is given by a function ϕ: $\{0, 1, 2, 3\} \to \{0, 1, 2, 3\}$; a particle approaching a vertex along edge j will leave that vertex along edge $\phi(j)$. The rules given are local, thus the particle will approach the next vertex along edge $\phi(j) + 2 \bmod(4)$. For each of the four incoming edges a scattering rule tells us on which of the four outgoing edges the particle will leave, thus there are $4^4 = 256$ scattering rules. Some special rules we will consider are a right rotator: $R(j) = j - 1 \bmod(4)$; a left rotator: $L(j) = j + 1 \bmod(4)$; and the straight-ahead rule: $S(j) = j + 2 \bmod(4)$. Another special pair of rules are $r(0) = 3$, $r(1) = 2$, $r(2) = 1$, $r(3) = 0$ and $l(0) = 1$, $l(1) = 0$, $l(2) = 3$, $l(3) = 2$, which are referred to as right and left mirrors (Fig. 1). The finite automaton is then an ordered set of scattering rules: $\{\phi_1, \phi_2, ..., \phi_k\}$.

A single particle with unit speed and four possible directions flows along the bonds of the lattice. When it enters the finite automaton in state $\phi_i \in \{\phi_1, \phi_2, ..., \phi_k\}$ it leaves it in state $\phi_{i+1 \bmod(k)}$. We will always assume

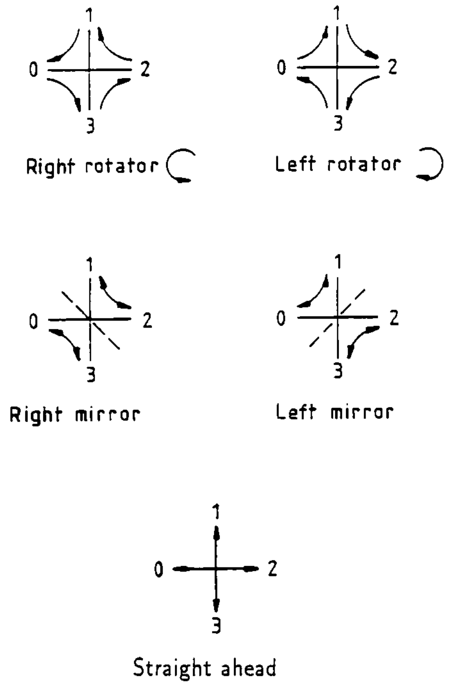

Fig. 1. A right rotator, a left rotator, a right mirror, a left mirror, and the straight-ahead rule.

that the cyclic group $\{\phi_1, \phi_2, ..., \phi_k\}$ is minimally presented, i.e., there is no $1 \leqslant l < k$ such that $\phi_i = \phi_{i+l \bmod (k)}$ $\forall i \in \{1, 2, ..., k\}$. For example, the cyclic group $\{L, R, L, R\}$ minimally presented is $\{L, R\}$. We consider all possible configurations of initial states Ω_0 on $\mathbf{Z}^2$, that is, $\Omega_0 = \{\phi_1, \phi_2, ..., \phi_k\}^{\mathbf{Z}^2}$. We will also consider the configuration space Ω_1 in which not all lattice sites have a finite automaton, those that have no finite automaton have the straight-ahead rule. This rule does not change when the particle passes through it. However, in this framework some of the ϕ_i can also be the straight-ahead rule, but they change their state to $\phi_{i+1 \bmod (k)}$ when a particle passes through the finite automaton. The enlarged configuration space is $\Omega_1 = \{S, \phi_1, \phi_2, ..., \phi_k\}^{\mathbf{Z}^2}$.

We discretize the flow by keeping track of the particle as it leaves vertices. Let $Z_i := \Omega_i \times \{0, 1, 2, 3\} \times \mathbf{Z}^2$ for $i \in \{0, 1\}$ be the phase space of the cellular automaton. A point $z = (\omega, d, (i, j)) \in Z_i$ consists of the configuration of states $\omega \in \Omega_i$, the velocity direction $d \in \{0, 1, 2, 3\}$ of the particle, and the location $(i, j) \in \mathbf{Z}^2$ of the particle. We denote by $g: Z_i \to Z_i$ the discretized motion.

We call the orbit of a point $z \in Z_i$ closed (periodic) if there is a positive integer n such that $g^n(z) = z$. We want to know the automata for which g will have at least one closed orbit.

A scattering rule ϕ is said to have no backscattering if $\phi(j) \neq j$ for all $j \in \{0, 1, 2, 3\}$. Our first theorem says that among all scattering rules without backscattering, only rotators can have closed orbits.

Theorem 1. For any $k \geqslant 1$ if for some $i \in \{1, 2, ..., k\}$ the scattering rule ϕ_i has no backscattering and there is a $z \in Z_1$ whose orbit is closed (periodic), then ϕ_i is a rotator (i.e., $\phi_i = L$ or $\phi_i = R$).

It is not hard to build counterexamples to Theorem 1 if we drop the assumption of backscattering.

We introduce two special models for $k = 2$. If $\phi_1 = R$, $\phi_2 = L$, the model is called the flipping rotator (FR) model and was introduced by Langton[7] and independently by several other authors. If $\phi_1 = r$, $\phi_2 = l$, the model is called the flipping mirror (FM) model and was introduced by Ruijgrok and Cohen.[4] As a corollary to Theorem 1, we have:

Corollary 2. Fix $k \geqslant 1$. Suppose for all $1 \leqslant i \leqslant k$ the scattering rules ϕ_i have no backscattering. If additionally there is a $z \in Z_1$ whose orbit is closed, then each ϕ_i is a rotator. In particular, if $k = 2$ and $\phi_1 \neq \phi_2$, the g is the FR model on Z_1, i.e., $\phi \equiv L$, $\psi \equiv R$ or vice versa.

Closed orbits for the FR model on Z_1 were discovered by Wu and Cohen.[5] In ref. 8 we showed that the FR model has no closed orbits in Z_0. The proof of this fact easily extends in our setting to the following theorem:

Theorem 3. For any $k \geqslant 1$ if for all $1 \leqslant i \leqslant k$ the scattering rules ϕ_i have no backscattering, then there is no $z \in Z_0$ whose orbit is closed.

To state the next theorem, we need a further definition. The transformation g is time reversible iff $\phi_i \equiv \phi^{-1}_{i+1 \bmod(k)}$ $\forall i \in \{1, 2,..., k\}$. Note that g can be time reversible only if $k = 2$! The models of this sort studied by physicists and chemists have all been of the sort $k = 2$. In this case we have the following additional result.

Theorem 4. If g is not time reversible and all ϕ_i do not have any backscattering, then g has no closed orbits.

The following corollary to Theorem 4 was proven in ref. 8.

Corollary 5. The FM model has no closed orbits.

From the previous theorems it is clear that the FR model plays a very special role among all cyclic cellular automata. The next theorem shows that it has very many closed orbits.

Theorem 6. Consider the FR model.

(a) (Full occupancy) Each $z \in Z_0$ has unbounded (and thus not closed) orbit.

(b) (Partial occupancy) Let μ be any product probability measure on Ω_1 with full support. Then the set $\{x \in \Omega_1$: the orbit of the particle starting at the origin (in any of the four directions) is closed$\}$ has full μ-measure.

(c) The set $\{x \in \Omega_1$: the orbit of the particle starting at the origin (in any of the four directions) is closed$\}$ is open and dense in Z_1.

Part (a) was proven in ref. 8.

When an orbit is periodic the past history of the trajectory determines the future; thus as a corollary to Theorem 6 we have:

Corollary 7. If μ is an invariant measure, then the entropy[12] of the FR model is zero.

Let $P(\mathbf{r}, n)$ be the probability density to find the particle at position $\mathbf{r} \in \mathbf{Z}^2$ at time n when it started at the origin at time $n = 0$ with each of the original four directions having equal probability. The main square displacement of the particle is then

$$\Delta(n) := \sum_{\mathbf{r} \in \mathbf{Z}^2} |\mathbf{r}|^2 P(\mathbf{r}, n) \tag{1}$$

The cellular automata is said to have a complete absence of diffusion if there is a constant C such that $\Delta(n) < C\ \forall n$.

Theorem 8. For any product probability measure on Ω_1 with full support, the FR model has a complete absence of diffusion.

Theorem 8 should be compared to a result in ref. 9, where for each $\varepsilon > 0$ an invariant measure is constructed for a certain Lorentz lattice gas cellular automaton for which almost every orbit is periodic but $\Delta(n) > n^{2-\varepsilon}$.

Let $X_i := \Omega_i \times \{0, 1, 2, 3\}$ for $i \in \{0, 1\}$. On X_i we think of the lattice site where the particle is located as the orogin and denote the discretized motion by $f\colon X_i \to X_i$. In this frame the motion is related to the particle's frame of reference. f is referred to as the Lagrangian dynamics, while the nonrelativized motion g is then called the Eulerian dynamics. Closed (periodic) Eulerian-g-orbits are always periodic Lagrangian-f-orbits, but the converse is far from being true.

In ref. 10 we studied periodic Lagrangian orbits for the FM model on X_0 or X_1 and the FR model on X_0. If μ gives equal mass to left and right rotators and each initial direction $\{0, 1, 2, 3\}$, then μ is an invariant measure for the Lagrangian dynamics f. Theorems 6 and 8 do not require the invariance of μ.

3. PROOFS OF RESULTS

The arithmetic of all scattering rules is mod(4) and this will not be explicitly stated in the proofs. A closed orbit defines a connected set $O \subset \mathbf{Z}^2$ of the vertices and edges which the particle hits and this set has a well-defined boundary $\Gamma := \partial O$. A corner of the boundary is a vertex with two edges in Γ and two edges in $\mathbf{Z}^2 \backslash O$, and for each of the pairs the two edges are perpendicular to each other. Clearly there are four possibilities for such corners.

Proof of Theorem 1. Since ϕ_i has no backscattering, the boundary of any closed orbit must have all four types of corners. Clearly the particle would have to hit each of the four corners when the scattering rule is in state ϕ_i. Because of this for each $j \in \{0, 1, 2, 3\}$ for each pair $j, j+1$ either $\phi(j) = j+1$ or $\phi(j+1) = j$. The proof is completed with the following lemma. ∎

Lemma A. If for each $j \in \{0, 1, 2, 3\}$, $\phi(j) = j+1$ or $\phi(j+1) = j$, then ϕ is a rotator.

Proof. Suppose $\phi(0)=1$. It is easy to see that if $\phi(1)=0$ or $=3$, the assumptions of the lemma cannot hold. Thus, $\phi(1)=2$. Likewise the assumption forces $\phi(2)=3$ and then $\phi(3)=0$, a left rotator. If originally $\phi(1)=0$, a right rotator arises. ▮

Proof of Theorem 4. Suppose g has a closed orbit. Since $\forall i \in \{1, 2\}$, ϕ_i has no backscattering, Theorem 1 implies that all rules are rotators. The minimal presentation of the finite automaton implies that $\phi_1 \neq \phi_2$ and thus one is a left rotator and the other is a right rotator. Thus g is time reversible, a contradiction. Thus no closed orbit could have existed. ▮

Proof of Theorem 6. (a) This part was proved in ref. 8.

(b) The special configuration drawn in Fig. 2 plays an important role in the creation of closed orbits. It is a "reflector," that is, when the particle enters it in the location and direction indicated in Fig. 2 it will leave it from the same location with the opposite direction. The configuration of rotators will be different at this moment, but they will have the same property. Namely, when the particle reenters at the same location in the same direction it will again exit the reflector from that location in the opposite direction. After the second time the configuration of rotators returns to the original configuration. Note that other configurations than the one of Fig. 2 (larger ones) can also be reflectors. Now any orbit which hits two nonintersecting reflectors will necessarily be closed, since the FR model is time reversible. Thus, to prove Theorem 6, we must show that for almost every configuration the particle starting at the origin will hit two different reflectors unless it is already periodic for some other reason.

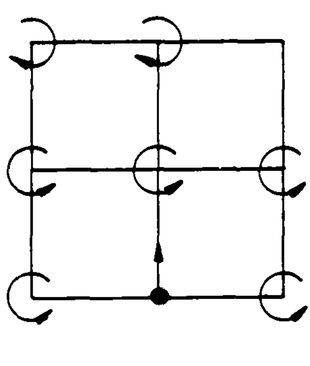

Fig. 2. A reflector.

To see this, we construct 20 different cylinder sets defined on 5 by 5 squares. Each of these cylinder sets has the reflector of Fig. 2 in the middle 3 by 3 square. The cylinder sets are so constructed that a particle entering into the cylinder set on a certain fixed edge will get reflected by the reflector. Two examples are shown in Fig. 3. Each of the cylinder sets will have this property for a different edge entering the square. Let $a > 0$ be the minimum of the measures of these 20 cylinder sets. Now periodically partition $\mathbf{Z}^2$ into 5 by 5 squares. Then the orbit of a particle will infinitely often cross from one box into another. Each time it enters a new box the probability it will enter a reflector is larger than a. If it enters only a finite number of new boxes, its orbit must be closed. Since the contents of newly entered boxes are independent, the Borel–Cantelli lemma implies that the particle will enter a reflector infinitely often with probability one. This implies that the orbit is closed.

(c) The density follows from part (b). Each closed orbit defines a cylinder set by fixing the states on the set of vertices which the orbit hits. All points in this cylinder set clearly have closed orbits. Each point whose orbit is closed is contained in such a cylinder set, and since cylinder sets are open, part (c) follows. ∎

Proof of Theorem 8. Let $B_n := \{(i, j) \in \mathbf{Z}^2: \max(|i|, |j|) \leqslant n\}$. Now, just as in Theorem 6, periodically partition $\mathbf{Z}^2$ into 5 by 5 boxes. For each of the 20 entering edges into a 5 by 5 box consider the set of all 5 by 5 configurations for which the configuration is not a reflector for the given entering edge. Call this set of configurations C_i (here i a label for the entering edge). Let $D_i := \{L, R, S\}^{B_5} \setminus C_i$, that is, the set of all 5 by 5 configurations which are reflectors for the given entering edge. Let $c_i := \mu(C_i)$. It is easy to see that C_i is nonempty and that D_i is also nonempty; thus $c_i \in (0,1)$. Let $c := \max_i c_i$. Since there is only a finite number of i, we have $c \in (0, 1)$ and

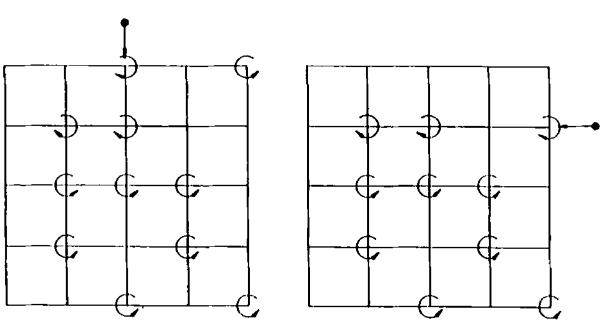

Fig. 3. A particle entering the 5 by 5 configuration along the indicated edge will be reflected by the reflector.

c is an upper bound on the probability that on entering a given 5 by 5 box we leave it without being reflected by a reflector.

We consider the set of periodic orbits that stay inside B_{5n} and are periodic because they hit two (special) nonintersecting reflectors, $R_{5n} := \{z \in Z_1$: among the first n different partition elements (5 by 5 boxes) which z's forward orbit visits, it encounters a reflector inside one of the elements (i.e., an event D_i), the same happens for z's backward orbits, and the partition elements where the forward and backward reflectors occur are distinct$\}$. Note that R_{5n} does not include z's which are periodic because they hit 5 by 5 reflectors at least one of which is not in the interior of a partition element of $\mathbf{Z}^2$ into 5 by 5 boxes, because they hit larger ($m \times m$, $m > 5$) reflectors or because they are periodic for some other reason. The orbits of $z \in R_{5n}$ visit at most $5 \times 5 \times 2n = 50n$ lattice sites. There are three scattering rules (L, R, S) and four directions; thus, it is not hard to see that the particle must have period less than or equal to $4 \cdot 3^{(50n)}$.

Let $P_n := \{z \in Z_1$: period $z = n\}$, $Q_n := \{z \in Z_1$: period $z \leqslant n\}$, $p_n := \mu(P_n)$, $q_n := \mu(Q_n)$, and $r_n := \mu(R_n)$. We have shown that $R_{5n} \subset Q_{4 \cdot 3^{(50n)}}$ or

$$r_{5n} \leqslant q_{4 \cdot 3^{(50n)}} \tag{2}$$

Let $R_{5n}^c := A_n^1 \cup A_n^2 \cup A_n^3$, where A_n^1 consists of the orbits not in R_{5n} which visit less than n different 5 by 5 boxes (i.e., they are periodic), A_n^2 consists of the orbits where either the forward or the backward orbit does not hit the appropriate reflector in the first n different boxes it visits, and A_n^3 consists of the orbits where both the forward and backward orbit hit only one reflector in the first n different boxes they visit and these reflectors intersect one another.

The measure A_n^2 is clearly bounded from above by $K_1 c^n$, where $K_1 > 0$. The measure of A_n^3 is bounded from above by $K_2 c^{n-1}$ ($K_2 > 0$), since both the forward and backward orbits have C_i-events $n-1$ times. Now it is not hard to see that in fact $Q_{4 \cdot 3^{(50n)}}^c \subset A_{5n}^2 \cup A_{5n}^3$. Thus, combining the above estimates gives

$$1 - r_n \leqslant K_3 \tilde{c}^n \tag{3}$$

where $K_3 > 0$ and $\tilde{c} \in (0, 1)$. Now

$$p_n + q_{n-1} \leqslant 1 \tag{4}$$

Combining Eqs. (2)–(4) yields $1 - q_n \leqslant K_4 \hat{c}^{K_5 \log n}$, where K_4, $K_5 > 0$ and $\hat{c} \in (0, 1)$. Thus

$$\Delta(n) \leqslant \sum_n n^2 p_n \leqslant \sum_n n^2 (1 - q_{n-1}) \leqslant \sum_n n^2 K_4 \hat{c}^{K_5 \log n} < \infty \quad \blacksquare \tag{5}$$

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