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On Localization of Vorticity in Lorentz Lattice Gases

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We study the generalized deterministic Lorentz lattice gases, in a fixed as well as in varying environments, in lattices with dimensions $d \geqslant 3$. We show that bounded orbits ("vortices") in these models are often contained in some lower dimensional subsets ("vortex sheets") of these lattices.

KEY WORDS: Lorentz gas cellular automata; local scattering rules; time reversibility; vortices.

Lorentz lattice gases (LLG), both deterministic and stochastic ones, have been extensively studied recently.[1-4] In LLG the immovable particles (scatterers) are situated at the sites of some lattice and, more importantly, a light particle can move only along the bonds of this lattice. This makes these models more restrictive than the classical Lorentz gas.[5]

However, a more general class of Lorentz gas cellular automata (LGCA) has two important new features:

(1) In LGCA different scatterers are allowed, i.e., the scatterers placed at different sites can be different. It is worth recalling that in the Lorentz gas all immovable particles (scatterers) have the same shape of spheres as well as in the other classical modification of the Lorentz gas (Ehrenfest's wind-tree model[6]), where all scatterers are identical rhombuses.

(2) LGCA contain also self-consistent models (sometimes these models are called flipping models) where there is a feedback of moving particle(s) to the environment of randomly distributed scatterers. This makes the class of LGCA automata much richer than the class of standard Lorentz lattice gases with fixed environment. Furthermore, it allows not

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only for the traditional applications of LGCA to statistical mechanics and chemistry, but also for a theory of artificial life[7] and to a theory of computations.[8]

Observe that it makes sense to consider the self-consistent LGCA not only for the motion of a single particle (specimen), but also a simultaneous motion of several particles (species). In fact, in contrast to standard (non-self-consistent) LLG, in such models different particles (species) are involved in the nontrivial interactions because each particle (specimen) changes the environment in which other particles (species) live (move). One of the interesting new problems for self-consistent models is to study the dynamics in the space of all possible environments that can even be chaotic.[9] It was pointed out recently[10] that these models (especially the self-consistent ones) can also be useful in the analysis and interpretation of numerical simulations of PDEs.

The studies of deterministic LLG were only numerical and always restricted to two dimensions.[1-3,11] The main reason for that was the totally new character of these models compared, e.g., to various models of a random walk in a random environment. Deterministic LGCA deal with a *deterministic walk in a random environment*, which drastically changes the character of the dynamics of such models. Therefore, standard methods of study of random-walk-type models fail here. This is the main reason why there are only a few rigorous mathematical papers devoted to the analysis of the LGCA. All of these studies are restricted to lattices in dimension two, $d=2$.

The first mathematical paper[10] on high-dimensional, $d>2$, deterministic LGCA revealed a surprising new property of these systems. This property, which we call a localization of vorticity, means that in deterministic high-dimensional Lorentz lattice gases bounded orbits (vortices) are confined in subsets of a lower dimension than the dimension d of a lattice itself where the motion of particles is studied. The analogy between the bounded orbits in LGCA and vortices is natural because any such orbit eventually terminates in a periodic motion on some finite subset of a lattice (which can have a rather complex shape).

It was shown in ref. 10 that such a localization of vorticity occurs in all non-self-consistent LGCA on cubic lattices with dimension $d \geqslant 3$. The only class of self-consistent LGCA for which the localization of vorticity was also proven in ref. 10 is rather narrow and restricted to $d=3$. In this paper we give a simple proof that such localization occurs for all time-reversible self-consistent LGCA on cubic lattices with dimension $d \geqslant 3$. We give also sufficient conditions that ensure the localization of vorticity on any (not necessarily cubic) lattices.

Now we give the exact definition of LGCA. We start with the cubic lattice $\mathbb{Z}^d$ in $\mathbb{R}^d$, $d \geqslant 2$. A single particle with unit speed and $2d$ possible directions flows along the bonds of the lattice. When it reaches a vertex $z \in \mathbb{Z}^d$ it continues its motion in the direction defined by a state of z (a current local scattering rule or, simply, a current scatterer at z). In addition, at the moments when the particle leaves a vertex the latter acquires some (generally a new) state, i.e., a local flow (scatterer) in a vertex is changed by the passage of the particle.

In other words, each vertex $z \in \mathbb{Z}^d$ contains a finite automaton $\phi(z)$ which at a given moment can be in one of k states. A finite automaton in a given state represents a scattering rule (scatterer, a local flow) present at this moment in the vertex $z \in \mathbb{Z}^d$. Namely, in $\mathbb{Z}^d$, $d \geqslant 2$, label the $2d$ edges (directions) coming to each vertex as $0, 1, 2,..., 2d-1$. We assume that the parallel and identically oriented edges are labeled by the same number at all vertices of $\mathbb{Z}^d$ and that the edges labeled by j and $j+d \pmod{2d}$ are parallel and have the opposite orientation.

A scattering rule (scatterer) is given by a function ϕ: $\{0, 1,..., 2d-1\} \to \{0, 1,..., 2d-1\}$: a particle approaching a vertex along edge j will leave that vertex along edge $\phi(j)$. The scattering rules are local; thus the particle will approach the next vertex along the edge $\phi(j)+d \pmod{2d}$. Therefore for each of the $2d$ incoming edges a scattering rule also defines on which of the $2d$ outgoing edges the particle will leave. Thus the total number of scattering rules on the lattice $\mathbb{Z}^d$ equals $(2d)^{2d}$.

An automaton $\Phi(z)$ at any vertex $z \in \mathbb{Z}^d$ is an infinite sequence of scattering rules $\{\phi_1(z), \phi_2(z),..., \phi_n(z),...\}$. The dynamics of the system is defined as follows. A single particle with unit speed and $2d$ possible directions flows along the bonds of the lattice. When it enters a vertex $z \in \mathbb{Z}^d$ in a state $\phi_i(z)$ it gets scattered according to the scattering rule $\phi_i(z)$ and it leaves a vertex z in a state $\phi_{i+1}(z)$.

Denote by Φ the space of all possible infinite sequences $\{\phi_i\}$, $i = 1, 2,..., n,...$, where each ϕ_i is one of $(2d)^{2d}$ scattering rules. Then the configuration space Ω (the space of all *evolving* environments) of our dynamical system is the set of all mappings $\mathbb{Z}^d \to \Phi$.

We discretize the flow by keeping track of the particle as it leaves the vertices. Thus $W := \Omega \times \{0, 1,..., 2d-1\} \times \mathbb{Z}^d$ is the phase space of the cellular automaton under study. A point $w = (w, v, (i_1, i_2,..., i_d)) \in W$ consists of the configuration of states (environment) ω, the velocity direction $v \in \{0, 1,..., 2d-1\}$ of the particle, and the location $(i_1, i_2,..., i_d) \in \mathbb{Z}^d$ of the particle. We denote by g: $W \to W$ the discretized motion.

This system generalizes all models of deterministic LLG considered so far.[1-3,11,12] In fact we consider the most general LGCA on $\mathbb{Z}^d$, because there are no restrictions at all to a structure of sequences of local scattering rules (scatterers) $\{\phi_i(z)\}$, $i = 1, 2, ..., n, ...$. It was always assumed that only one or two nontrivial scattering rules are permitted and in the latter case these two scattering rules always alternate.[1-3,11] The trivial scattering rule (Fig. 1a) (straightahead; i.e., no scattering) together with the pair of left and right mirrors (Fig. 1c) or with the left and right rotators (local vortices) (Fig. 1b) were the only types of scatterers studied numerically (see, e.g., refs. 1–3 and 11).

All these models assume that in some vertices the scattering rule is trivial for all $i = 1, 2, ..., n, ...$ and in all other vertices the scattering rule is the same for all i or it is one for all odd i's and the symmetric one for all even i's. The generalization of these models was studied in ref. 12 where an arbitrary (but the same!) finite sequence of scatterers was cyclically repeated in all vertices with a nontrivial local scattering.

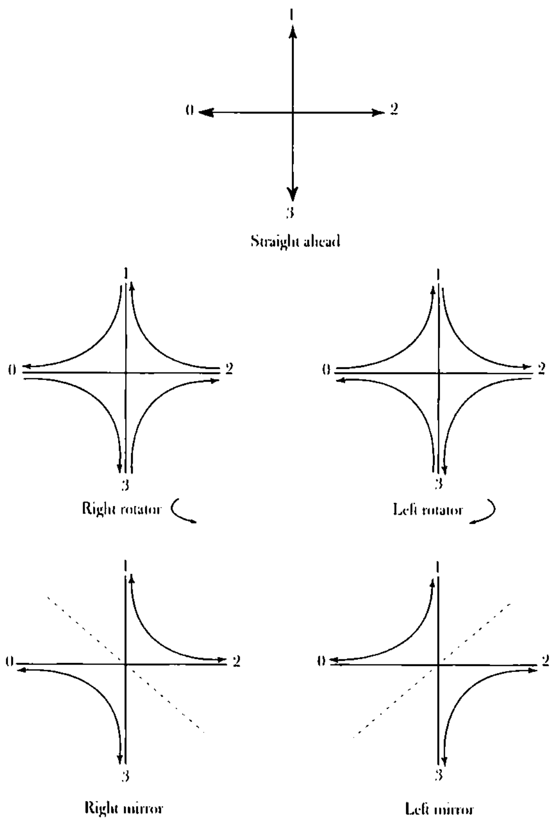

Fig. 1. (a) The trivial (straightahead) rule; (b) rotators; (c) mirrors.

We call the orbit of a point $w \in W$ *closed* (periodic) if there is a positive integer n such that $g^n(w) = w$. The orbit of a point $w \in W$ is called *bounded* if the particle visits only a finite number of vertices in the lattice $\mathbb{Z}^d$, i.e., $\pi\{g^n(w)\}$ is a finite set, where π: $W \to \mathbb{Z}^d$ is the natural projection of the phase space W into $\mathbb{Z}^d$.

Let $\{g^m(w)\}$, $m = 0, 1, 2,...,$ be a bounded orbit. Then $\pi\{g^m(w)\} = \{z_1, z_2,..., z_k\}$, where $z_i \in \mathbb{Z}^d$, $i = 1, 2,..., k$. We call a vertex z_i *essential* if $z_i = \pi g^r(w)$ for infinitely many r. Otherwise a vertex $z_i \in \mathbb{Z}^d$ will be called nonessential for a given bounded orbit $\{g^m(w)\}$.

The union of all essential vertices of a bounded orbit $\{g^m(w)\}$ will be called a core of this orbit and denoted as $\mathrm{Cor}\{g^m(w)\}$. Thus a core of a bounded orbit is the collection of all such vertices in $\mathbb{Z}^d$ that the orbit visits infinitely many times. Therefore one thinks of this motion as some kind of a vortex. Obviously a bounded orbit $\{g^m(w)\}$ spends a finite time outside its core.

It was shown in refs. 12 and 10 that in LGCA in $\mathbb{Z}^2$ the right and left rotators only can produce global vorticity, i.e., bounded orbits, among all scattering rules without backscattering.

The situation for LGCA on $\mathbb{Z}^d$, $d \geqslant 3$, is different. In this case there are many scattering rules that can produce vorticity (bounded motion). However, such "vortices" can fill in only some lower dimensional regions (Fig. 2).

Let $\{g^m(w)\}$ be a bounded orbit of an LGCA on some lattice. Consider the union of all bonds of this lattice such that both their ends belong to $\mathrm{Cor}\{g^m(w)\}$. We denote this set by $\mathrm{Sc}(g^m(w))$ and call it the skeleton of a bounded orbit $\{g^m(w)\}$.

Our first result deals with nonflipping (fixed scatterers) LGCA. (It is the generalization of Theorem 5 in ref. 10.)

Theorem 1. Let $\{g^m(w)\}$ be a bounded orbit of LGCA on $\mathbb{Z}^d$, $d \geqslant 3$, with a unique nontrivial local scattering rule ϕ. Then the skeleton of $\{g^m(w)\}$ cannot contain any polyhedron in $\mathbb{Z}^d$ that has a dimension greater than $[\log_2 d] + 1$, where $[\cdot]$ denotes an integer part of a number.

(Observe that Theorem 1 is trivially valid for $d = 2$, but it does not provide any information in that case because $[\log_2 d] + 1$ equals the dimension of a lattice.)

Proof. Suppose that $\mathrm{Sc}\{g^m(w)\}$ does contain a polyhedron P such that $\dim P = d_1 \geqslant \log_2 d + 1$. Then the total number of vertices of P is at least $2^{d_1} > 2d$.

The total number $c(\mathbb{Q})$ of oriented incoming edges at any vertex of a regular lattice $\mathbb{Q}$ is called the *coordination number* of this lattice. The coordination number of $\mathbb{Z}^d$ equals $2d$. Therefore there exist at least two different

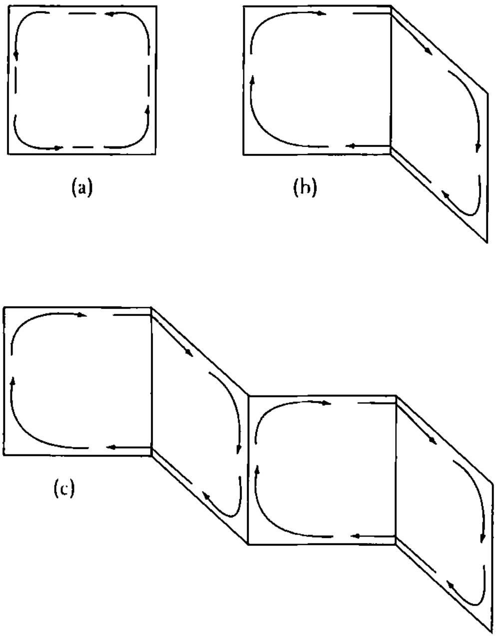

Fig. 2. Two-dimensional vortex sheets on the cubic lattice.

vertices $z_i \in P$, $i = 1, 2$, such that the orbit $\{g^m(w)\}$ arrives at z_1 and z_2 along two parallel and identically oriented bonds. However, the continuations of these paths that arrive at z_1 and z_2 always stay parallel because we have only one type of nontrivial scatterer (Fig. 3). Therefore they cannot belong to the same orbit. This contradiction proves the theorem.

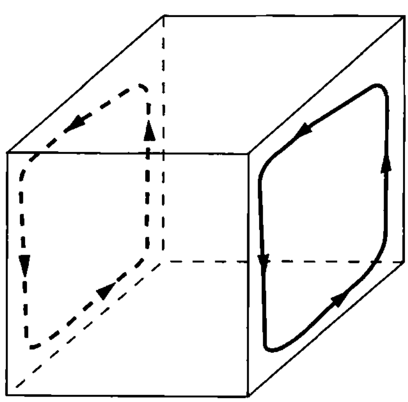

Fig. 3. Parallel velocities produce orbits confined to parallel planes.

Theorem 1 has the following corollary, which can be proven by the verbatim repeating of the above proof.

Corollary. Let $\{g^m(w)\}$ be a bounded orbit of an LGCA on some regular lattice $\mathbb{Q} \subset \mathbb{R}^d$ with a unique nontrivial scattering rule ϕ. Suppose that the number of vertices in a fundamental region of $\mathbb{Q}$ (elementary cell of a lattice) is greater than $2c(\mathbb{Q})$. Then the skeleton of $\{g^m(w)\}$ cannot contain any polyhedron in $\mathbb{Q}$ that has the dimension d.

Remark 1. Again, this corollary does not provide any information in the planar case.

Remark 2. An estimation of the maximal dimension for a skeleton of a bounded orbit can be made much more precise for concrete examples of lattices (as, e.g., in Theorem 1).

It is natural to ask whether or not the analogous localization of vorticity occurs in some self-consistent LGCA. We recall that these models should contain more than one type of nontrivial scatterer and the type of scatterer must change with time at all vertices with nontrivial scatterers.

Obviously, a self-consistent LGCA without any restrictions on possible types of scatterers does not have the property of localization of vorticity. Indeed, one can put at each vertex of any polyhedron such a sequence of scatterers that is specially prepared to fill in this polyhedron. However, this property holds for the important class of time-reversible LGCA. [For example, the flipping-mirrors (rotators) model is non-time-invertible (time-invertible).]

Theorem 2. Consider a self-consistent (flipping) LGCA on $\mathbb{Z}^d$, $d \geq 3$. Suppose that the dynamics is time-reversible. Then the skeleton of any bounded orbit cannot contain any polyhedron in $\mathbb{Z}^d$ with dimension greater than $[\log_2 d] + 1$.

Proof. Let $z \in \mathbb{Z}^d$ be some vertex. Denote by $\phi_t(z)$ a scatterer that is present at the vertex z at the moment t. It is easy to see that in a time-reversible LGCA $\phi_{t+1}(z) = \phi_t^{-1}(z)$. Therefore any time-reversible self-consistent LGCA contains exactly two nontrivial scattering rules that are inverse to each other.

Now Theorem 2 follows immediately from the proof of Theorem 1.

The analogous corollary of this theorem also holds.

Corollary. Let $\{g^m(w)\}$ be a bounded orbit of a time-reversible LGCA on some regular lattice $\mathbb{Q} \subset \mathbb{R}^d$. Suppose that the number of vertices in a fundamental region of $\mathbb{Q}$ is greater than $2c(\mathbb{Q})$. Then the skeleton of $\{g^m(w)\}$ belongs to some polyhedron in $\mathbb{Q}$ that has dimension strictly less than d.

Remark 3. One can substitute $2c(\mathbb{Q})$ by $c(\mathbb{Q})$ in the corollaries to Theorems 1 and 2 if the lattice $\mathbb{Q}$ consists entirely of straight lines.

So far we have considered the LGCA in infinite lattices. However, the same models can be considered in bounded subsets of lattices. We believe that the study of such models can also shed some light on the behavior of grid schemes in the numerical simulations of PDEs.

We will give now the exact definition of such models. For the sake of brevity we consider only cubic lattices.

Let $\mathscr{D} \subset \mathbb{Z}^d$ be a bounded subset of a lattice $\mathbb{Z}^d$. A point $z \in \mathscr{D} \subset \mathbb{Z}^d$ is an inner point of $\mathscr{D}$ if all its $2d$ nearest neighbors also belong to $\mathscr{D}$. We call $\mathrm{Int}(\mathscr{D})$ the collection of all interior points of $\mathscr{D}$. A boundary $\partial\mathscr{D} = \mathscr{D} \backslash \mathrm{Int}(\mathscr{D})$. One cannot choose arbitrarily local scattering rules at the points of $\partial\mathscr{D}$ because the particle is not permitted to leave $\mathscr{D}$. Keeping in mind this restriction, denote by $\Omega_{\mathscr{D}}$ the set of all admissible mappings (environments) $\mathscr{D} \to \Phi$ and by $W_{\mathscr{D}} := \Omega_{\mathscr{D}} \times \{0, 1,..., 2d-1\} \times \mathscr{D}$ the corresponding phase space, where $\{0, 1,..., 2d-1\}_{\mathscr{D}}$ denotes the set of admissible (at a given $z \in \mathscr{D}$) scattering rules.

Results analogous to Theorems 1 and 2 hold for LGCA in bounded regions, where one should substitute a "bounded orbit" by a "bounded orbit that does not intersect the boundary $\partial\mathscr{D}$." The corresponding proofs are completely analogous to the case of infinite lattices. Because of that we will only formulate the statement analogous to Theorem 1.

Theorem 1′. Let $\{g^m(w)\}$ be a bounded orbit of LGCA in $\mathscr{D} \subset \mathbb{Z}^d$, $d \geqslant 3$, with a unique nontrivial local scattering rule. Let, moreover, $\{g^m(w)\} \cap \partial\mathscr{D} = \phi$. Then the skeleton of $\{g^m(w)\}$ cannot contain any polyhedron in $\mathbb{Z}^d$ that has a dimension greater than $[\log_2 d] + 1$.

We believe that the results on the localization of bounded orbits ("vorticity") in subsets of lower dimensions ("vortex sheets") might have some applications for the analysis and interpretation of computer simulations of PDEs.

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