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ON THE ABSENCE OF HOMOGENEOUS SCALAR UNITARY CELLULAR AUTOMATA

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ABSTRACT

Failure to find homogeneous scalar unitary cellular automata (CA) in one dimension led to consideration of only "approximately unitary" CA—which motivated our recent proof of a No-go Lemma in one dimension. In this note we extend the one dimensional result to prove the absence of nontrivial homogeneous scalar unitary CA on Euclidean lattices in any dimension.

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A classical cellular automaton (CA) consists of a lattice L of *cells* together with a *field* $\phi : \mathbb{N} \times L \to S$, where $\mathbb{N}$ denotes the non-negative integers labelling timesteps and S is the set of possible *states* in which the field is valued. Time evolution is locally defined; in the special case of an *additive* CA the field evolves according to a *local rule* of the form:

$$\phi_{t+1}(x) = \sum_{e \in E(t,x)} w(t, x+e)\phi_t(x+e), \tag{1}$$

where $E(t,x)$ is a set of lattice vectors defining local *neighborhoods* for the automaton [1]. For the purposes of this note, the lattice L is taken to be generated by a set of d linearly independent vectors in $\mathbb{R}^d$, *i.e.*, as a group under vector addition L is isomorphic to $\mathbb{Z}^d$ or some periodic quotient thereof. If $E(t,x)$ is a constant neighborhood and $w(t, x+e) \equiv w(x+e)$, the CA is *homogeneous*. For example, in the $\mathbb{Z}^2$ lattice generated by v_1 and v_2, the neighborhood $E = \{0, \pm v_1, \pm v_2, \pm(v_1 + v_2)\}$ defines the "triangular lattice".

The additive evolution rule (1) is more compactly expressed as (left) multiplication of the vector ϕ_t by an *evolution* matrix having non-zero entries (the *weights* $w(t, x+e)$) in row x only in columns $x+e$ for $e \in E(t,x)$. For example, if S consists of the real numbers in the unit interval $[0,1]$, the weights $w(t, x+e)$ are positive, and the sum of the entries in each column of the evolution matrix is 1, then (1) defines a specific *probabilistic* CA [2]. The evolution preserves the L^1 norm of ϕ: $\sum_x \phi(x)$; if the L^1 norm of ϕ_0 is one, then $\phi_t(x)$ may be interpreted physically as the probability that the system is in state x at time t. If the lattice of cells is a discretization of space, as suggested by the locality of the evolution rule (1), $\phi_t(x)$ is naturally interpreted to be the probability that a stochastic particle is in cell x at time t.

If the field is complex valued, or more precisely, if $S = \{z \in \mathbb{C} \mid |z| \leq 1\}$, and the evolution matrix is *unitary* then (1) defines what we refer to here as a *scalar unitary* CA; this is a special case of a *quantum* CA (QCA) [3,4,5,6]. Unitary evolution preserves the L^2 norm of ϕ: $(\sum_x |\phi(x)|^2)^{1/2}$; if the L^2 norm of ϕ_0 is 1, then $\phi_t(x)$ is the *amplitude* for the system to be in, and $|\phi_t(x)|^2$ is the probability of observing, the state x at time t. Scalar QCA were first considered by Grössing and Zeilinger [4], although they found nontrivial homogeneous scalar CA in one dimension with neighborhoods of radius one (*i.e.*, with the evolution matrix tridiagonal) only by relaxing their definition to allow "approximately unitary" evolution. In [3] we showed that only trivial homogeneous scalar unitary CA exist in one dimension with neighborhoods of *any* size:

NO-GO LEMMA. *In one dimension there exists no nontrivial, homogeneous, scalar unitary CA. More explicitly, every band r-diagonal unitary matrix which commutes with the 1-step translation matrix is also a translation matrix, times a phase.*

The purpose of this note is to show that the analogous result also holds in higher dimensions. This will be important when we extend the one dimensional models of [3] to more realistic simulations of two or three dimensional systems [7]. We shall give two different proofs of this No-go Theorem and then conclude by explaining how it may be evaded in order to find nontrivial QCA in any dimension.

Consider first a lattice $L = \mathbb{Z}_{n_1} \oplus \cdots \oplus \mathbb{Z}_{n_d}$, *i.e.*, a finite lattice which is locally isomorphic to $\mathbb{Z}^d$ but is periodic in each coordinate. The cells of this lattice may be ordered lexicographically by their coordinates: for a cell $(x_1, \ldots, x_d)$,

$$x := x_d + n_d\, x_{d-1} + n_d n_{d-1}\, x_{d-2} + \cdots + n_d \ldots n_2\, x_1 \tag{2}$$

defines the position of the cell in a one dimensional array. In a CA with a neighborhood of radius r the value of the field at this cell depends on the values of the field at the cells $\{(y_1, \ldots, y_d) \mid |x_i - y_i| \le r\}$ at the previous timestep. In the representation defined by (2), the evolution matrix U is what we may describe as "depth d band r-diagonal" (the more familiar "tridiagonal with fringes" matrix arising in the finite difference method solution to a second order elliptic equation in two variables [8] is depth 2 band 1-diagonal in this terminology). More importantly for our purposes, U is (sparsely) band Kr-diagonal, where

$$K := 1 + n_d + n_d n_{d-1} + \cdots + n_d \ldots n_2,$$

as shown in Figure 1.

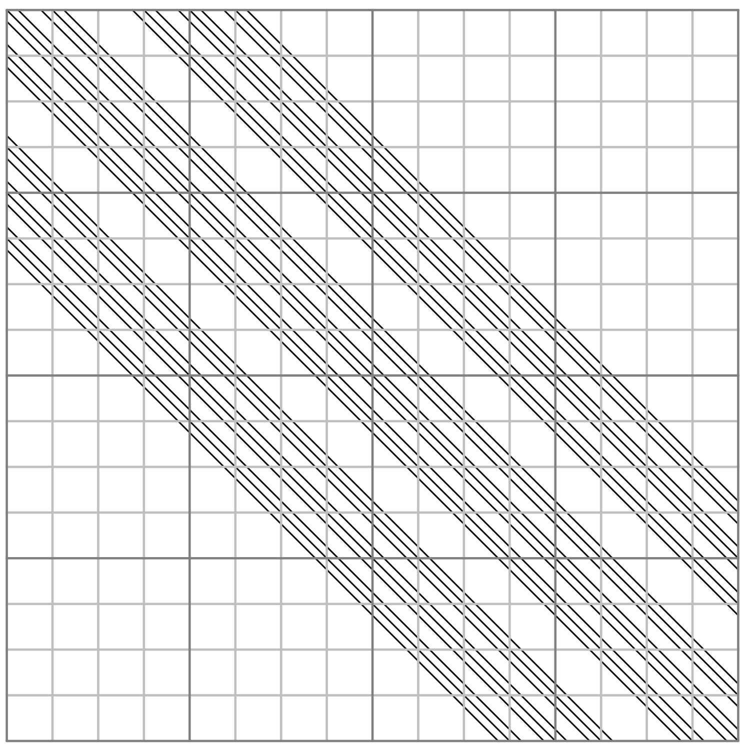

Figure 1. A portion of the depth 3 band 1-diagonal evolution matrix U for the lattice with dimensions (n_1, n_2, n_3). The small grey squares have size $n_3 \times n_3$; there are $n_2 \times n_2$ grey squares in each medium black square; and there are $n_1 \times n_1$ black squares in the whole array. U is band $1(1 + n_3 + n_3 n_2)$-diagonal.

The product of two band Kr-diagonal matrices is necessarily band $2Kr$-diagonal. The proof of the one dimensional No-go Lemma given in [3] depends only on the size of U being large enough that the band $2Kr$-diagonal product $UU^\dagger$ is still band diagonal, namely that

$$1 + 4Kr \leq n_d \dots n_1. \tag{3}$$

Given any r, for a sufficiently large lattice L (specifically, for sufficiently large n_1), inequality (3) is satisfied.

The conclusion of the argument in [3] is that the only band diagonal solution to $UU^\dagger = I$ is a phase times a matrix with only non-zero entries being ones along a single diagonal within the band. This is a translation matrix even in the present higher dimensional context. Thus, as a scholium to the No-go Lemma for homogeneous scalar unitary CA in one dimension, we have proved:

NO-GO THEOREM. *In any dimension the only homogeneous, scalar unitary CA evolve by a constant translation with overall phase multiplication.*

Although the proof just given is straightforward, the physical and geometrical content of the result is perhaps obscured by the unraveling of the higher dimensional lattice L into the one dimensional representation (2). In fact, the theorem does not depend on the finiteness of the lattice which was necessary for the band diagonality of the U shown in Figure 1. To rectify this problem let us consider a second argument using a sum-over-histories approach. In [3] we saw that this is particularly natural since a scalar QCA may be interpreted to be a quantum particle automaton: the system consists of a single particle moving on the lattice, $\phi_t(x)$ is the amplitude for the particle to be in state x at time t, and the weight $w(t, x+e)$ is the amplitude for the particle to move from $x + e$ to x.

In the sum-over-histories framework for quantum mechanics a probability is associated to a set S of particle histories (defined by boolean expressions in projectors onto states x_i at times t_i) by the rule:

$$|S| = \sum_{\gamma_1,\gamma_2 \in S} w(\gamma_1)\overline{w}(\gamma_2)\delta\big(\gamma_1(T), \gamma_2(T)\big),$$

where the delta function ensures that the only non-zero contributions to the probability come from pairs of paths in S which coincide at the *truncation time* T [9]. Of course, as shown in Figure 2, only truncation times defining spacelike hypersurfaces entirely to the future of the conditions defining S are permitted. *Unitarity is the invariance of probability under a change in truncation time.* That is, for

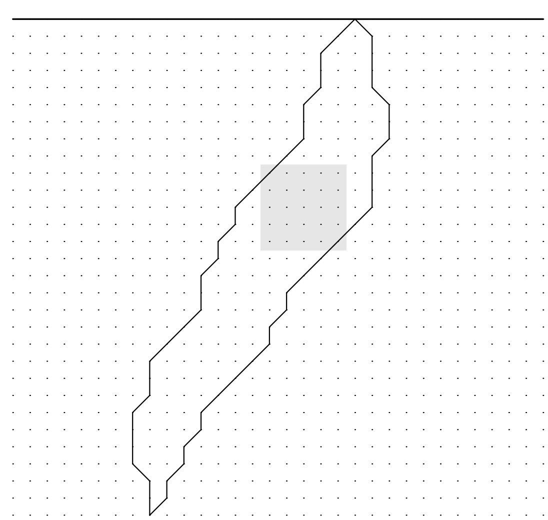

Figure 2. A pair of spacetime histories of the quantum particle in a one dimensional automaton with local neighborhood of radius 1 in the set S defined by intersection with the shaded region R of spacetime. Since the histories coincide at the truncation time (which lies to the future of R), they contribute to the probability $|S|$.

any two states x_1 and x_2, the sum of the contributions of all pairs of paths, one from each of these states at time T_1 to any common state x at time $T_2 > T_1$, must vanish unless $x_1 \equiv x_2$, in which case it must be one.

In particular, this condition applies to the paths corresponding to advancing the truncation time by one timestep. In a homogeneous CA, a cell x_1 may influence cells in the constant neighborhood E around it at the next timestep; hence any pair of paths, one from each of x_1 and x_2, which coincide at the next timestep, do so at a cell in the intersection of the neighborhood around x_1 and the neighborhood around x_2. The unitarity conditions on the weights in (1) thus arise from each pair of cells with intersecting neighborhoods: the corresponding sum vanishes except when the two cells coincide, in which case it is one.

With this description of the unitarity conditions it is easy to prove the No-go Theorem. Order the cells in the neighborhood of x_1 as in (2). Let k be the position of the first non-zero weight w_k in this ordering (there must be one since the zero matrix is not unitary) and let e_k denote the corresponding lattice vector. Consider $x_2 := x_1 + e_{|E|} - e_k$. The set of cells with possibly non-zero weights in the neighborhood of x_2 intersects the neighborhood of x_1 only at the last cell in that ordering, so $w_k \overline{w}_{|E|} = 0$ and hence $w_{|E|} = 0$. Now slide the second neighborhood down one as in Figure 3, *i.e.*, let $x_2 := x_1 + e_{|E|-1} - e_k$. The set of cells with possibly non-zero weights in the intersection of x_1 and x_2 is again a singleton, still labelled k in the neighborhood of x_2, but now $|E| - 1$ in the neighborhood of x_1. So $w_k \overline{w}_{|E|-1} = 0$ and hence $w_{|E|-1} = 0$. Continue this process until $x_2 = x_1$, whence unitarity requires $w_k \overline{w}_k = 1$. The conclusion of the No-go Theorem follows: the one step evolution of this homogeneous scalar unitary CA is translation by e_k and multiplication by the phase w_k.

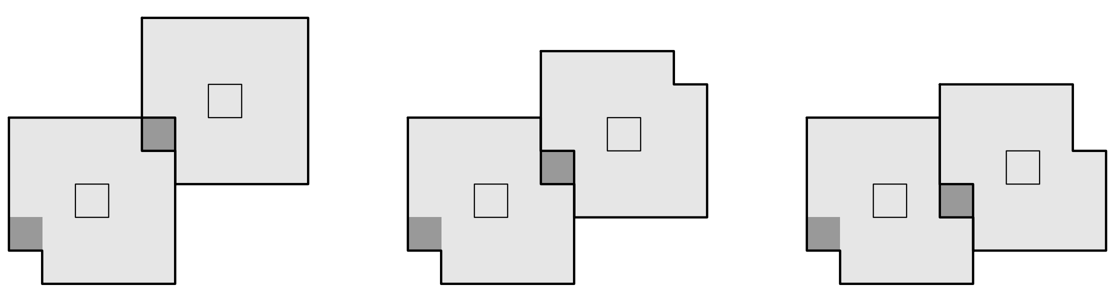

Figure 3. Intersecting neighborhoods of radius 2 in a two dimensional CA; in each pair x_1 is the lower left cell outlined and x_2 is the upper right one. The first non-zero weight is at position 2 (dark grey) in each neighborhood. In the three steps of the argument shown, x_2 is shifted so that the cell at position 2 in its neighborhood coincides successively with the cell at position $|E| = 25$, then 24, then 23 in the neighborhood of x_1. When the last column has been depleted the process is repeated on the next to last, *etc.*, until the neighborhoods coincide.

The homogeneity hypothesis in the No-go Theorem is the requirement that the evolution matrix be invariant under the action of the translation group of the lattice. The conclusion is that this restriction on scalar unitary CA renders them too simple to be of much interest. As we showed in [3], however, if the evolution matrix is required to be invariant only under the action of a subgroup of the translation group of the one dimensional lattice, the No-go Lemma is evaded and there are many interesting scalar QCA (the first of which seems to have been described by Feynman [10]; similar discrete models for a quantum particle have been studied by several authors more recently [5,11]). This is equally true in higher dimensional lattices: the one step evolution of a quantum *partitioning* [2,12] CA is invariant under the action of a subgroup of the translations on the lattice and may be interpreted to be composed of particle scattering matrices. Higher dimensional quantum particle automata [7,13] and their generalizations to quantum lattice gas automata [7,14] have been constructed in exactly this way.

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