Reversible Quantum Cellular Automata

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We define quantum cellular automata as infinite quantum lattice systems with discrete time dynamics, such that the time step commutes with lattice translations and has strictly finite propagation speed. In contrast to earlier definitions this allows us to give an explicit characterization of all local rules generating such automata. The same local rules also generate the global time step for automata with periodic boundary conditions. Our main structure theorem asserts that any quantum cellular automaton is structurally reversible, i.e., that it can be obtained by applying two blockwise unitary operations in a generalized Margolus partitioning scheme. This implies that, in contrast to the classical case, the inverse of a nearest neighbor quantum cellular automaton is a nearest neighbor automaton.

We present several construction methods for quantum cellular automata, based on unitaries commuting with their translates, on the quantization of (arbitrary) reversible classical cellular automata, on quantum circuits, and on Clifford transformations with respect to a description of the single cells by finite Weyl systems. Moreover, we indicate how quantum random walks can be considered as special cases of cellular automata, namely by restricting a quantum lattice gas automaton with local particle number conservation to the single particle sector.

I. INTRODUCTION

The idea of generalizing the classical notion of cellular automata to the quantum regime is certainly not new. Indeed, it is already present in Feynman’s famous paper from 1982, in which he argues that quantum computation might be more powerful than classical. However, although there have been several formal definitions of quantum cellular automata over the years, the theory is not in good shape at the moment, and a systematic exploration of the general properties of such systems on the one hand and of the potential for computational applications on the other has hardly begun. We believe that this is partly due to deficiencies of the existing approaches, and therefore propose a new one, which is very natural, and only requires a few basic assumptions: a discrete cell structure with a finite quantum system for every cell and translation symmetry, a discrete time step for the global system, reversibility, and finite propagation speed.

Quantum cellular automata (“QCAs”) are of interest to several fields. There are obvious connections to the statistical mechanics of lattice systems, and potential applications to ultraviolet regularization of quantum field theories. In Quantum Computer Science they appear as one natural model of computation extending the well-developed theory of classical cellular automata into the quantum domain. But also the experimental side is rapidly developing: quantum computing in optical lattices and arrays of microtraps are among the most promising candidates for the first quantum computer that does useful computations. It is typical for such systems that the addressing of individual cells is much harder than a change of external parameters affecting all cells in the same way. But this is just the theoretical description of a cellular automaton. Possible tasks, which have the same built-in translation invariance are simulations of solid state models. Typically classical simulations run into problems already for moderate systems sizes, precisely because of the dimension and complexity explosion which Feynman noted, and for which he proposed quantum computation as a cure. The theory presented in this paper can be considered as providing the first elements of an assembly language for such simulations.

The problems which have plagued previous attempts to define QCAs begin with the definition of a system of infinitely many cells. Consider the simplest operation such an automaton should be able to perform: applying the same unitary transformation separately to each cell. This would involve multiplying infinitely many phases, so there is really no well-defined unitary operator describing the global state change. Therefore, the quantization approach “just make the transition function unitary” does not work very well. Similarly, the notion of state vectors as amplitude assignments to uncountably many classical configurations is ill-defined. But this would be a candidate for the “configurations” of a QCA, which causes problems for a definition of QCAs in terms of configurations and their transformations. Various approaches will be described and commented in Section V. A constructive method to obtain QCAs, which is common to most of these approaches (including ours) is partitioning the system into blocks of cells, applying blockwise unitary transformations, and possibly iterating such operations. Model studies based on such construc-
tions (e.g., [10]) therefore produce results independently of the definition problems.

In order to arrive at a satisfactory notion of QCAs, it is helpful to draw on ideas from a discipline, which has been dealing with infinite arrays of simple quantum systems for a long time, i.e., the statistical mechanics of quantum spin systems. Infinite systems have been considered particularly in the algebraic approach to such systems [11]. The basic idea is to focus on the observables rather than the states, i.e., to work in the Heisenberg picture rather than the Schrödinger picture [12]. The main advantage is that in contrast to localized states, it does make sense to speak of local observables [13], i.e., observables requiring a measurement only of a finite collection of cells. The global transition rule of a cellular automaton is then a transformation $T$ on the observable algebra of the infinite system. As always in the Heisenberg picture, the interpretation of such a transformation is that 'preparing a state, running the automaton for one step, and then measuring the observable $A$' gives exactly the same expectations as preparing the same state and measuring $T(A)$. As always, $T$ must be completely positive and satisfy $T(1) = 1$. But more importantly we can state the crucial localization property of QCAs: When $A$ is localized on a region $\Lambda$ of the lattice, then $T(A)$ should be localized in $\Lambda + \mathcal{N} = \{ x + n \mid x \in \Lambda, n \in \mathcal{N} \}$, where $\mathcal{N}$ is the neighborhood scheme of the QCA.

To our knowledge, this view of QCAs was first used in [14], where the approach to equilibrium in a QCA with irreversible local rules (based on a partitioning scheme) was investigated. The general picture of QCAs remained unsatisfactory, however, because the partitioning scheme seemed a rather special way of constructing a QCA. For a satisfactory theory of QCAs we demand that there should be a direct connection between the global transition rule $T$ and the local transition rule: If we know the global transition rule, we should be able to extract immediately the local rule in a unique way, and conversely, from the local rule we should be able to synthesize the global rule. The class of global rules should have an axiomatic specification, the most important of which would be the existence of a finite neighborhood scheme in the above sense. On the other hand, for the local transition rules we would prefer a constructive characterization. That is, there should be a procedure for obtaining all local rules leading to global rules with the specified properties, in which all choices are clearly parameterized.

The partitioning QCAs of [14] failed to meet these requirements, because they provided a construction, but no axiomatic characterization of the global rules obtained in this way. In particular, it remained unclear whether two steps of such an automaton could be considered as a single step of an automaton with enlarged neighborhood scheme. The idea enabling the present paper was that all these difficulties vanish if we restrict to the class of reversible QCAs. The axiomatic characterization is extremely simple: In addition to the above locality condition we assume that the global rule must have an inverse, which is again an admissible quantum channel. This is equivalent to saying that $T$ must be an automorphism of the observable algebra. Then the local rule is simply the restriction of this automorphism to the algebra of a single cell. Conversely, since every observable can be obtained as a linear combination of products of single-cell observables, the local rule determines the global automorphism. This allows us to subsume all the known constructions of QCAs, but also to prove a general structure theorem: every reversible QCA is structurally reversible, i.e., we can write the local rule in a partitioning scheme involving two unitary matrices, which makes it apparent how the global rule can be unitarily implemented on arbitrarily large regions, and how to obtain the local rule of the inverse.

A further bonus from our proof of the structure theorem is that it does not actually require the global rule to be an automorphism: it works under the prima facie much weaker assumption that the global rule is a homomorphism (and not necessarily onto). Then invertibility follows (see Corollary 1 below). Therefore, invertibility was not included in Definition 1, which makes it much easier to verify whether a proposed rule is indeed a QCA.

The structural invertibility was an open problem in the theory of classical reversible cellular automata in higher dimensional lattices until recently [15]. Hence, since our proof of the quantum result is rather simple, it appears that some proofs in the classical domain can be simplified by going quantum.

Our paper is organized as follows: In Section II we begin with the axiomatic definition of QCAs in the sense described above. Its counterpart, the constructive description is given in the form of a collection of basic constructions and examples in Section III. It turns out that one of these constructions, based on partitioning, is already sufficient to obtain all QCAs in the sense of our definition. This rather surprising result is stated and proved in Section V. The ideas of the proof also allows us to give an explicit parameterization of the simplest class of QCAs: nearest neighbor automata in one dimension with one qubit per cell. As mentioned in the introduction, the current literature on the subject is mostly based on a definition we do not find satisfactory. We discuss these, and some further related definitions, in more detail in Section VI. Finally, in an appendix we provide some mathematical background on finite dimensional C*-algebras, which play a key role in the proof of Theorem 5.

II. DEFINITION OF QCAS

We consider an infinite cubic array of cells, labelled by integer vectors $x \in \mathbb{Z}^s$, where $s \geq 1$ is the spatial dimension of the lattice [16]. Each cell contains a $d$-level quantum system with the same finite $d \geq 2$. That is to say, with each cell $x \in \mathbb{Z}^s$, we associate the observable algebra $A_x$ of the cell, and each of these algebras is an isomorphic copy of the algebra of complex $d \times d$-matrices.
When $\Lambda \subset \mathbb{Z}^d$ is a finite subset, we denote by $\mathcal{A}(\Lambda)$ the algebra of observables belonging to all cells in $\Lambda$, i.e., the tensor product $\bigotimes_{x \in \Lambda} \mathcal{A}_x$. By tensoring with unit operators on $\Lambda_2 \setminus \Lambda_1$ we consider $\mathcal{A}(\Lambda_1)$ as a subalgebra of $\mathcal{A}(\Lambda_2)$, whenever $\Lambda_1 \subset \Lambda_2$. In this way the product $A_1 A_2$ of $A_i \in \mathcal{A}(\Lambda_i)$ becomes a well-defined element of $\mathcal{A}(\Lambda_1 \cup \Lambda_2)$. Moreover, tensoring with the identity does not change the norm, so we get a normed algebra of local observables, whose completion is called the quasi-local algebra $\mathcal{A}(\mathbb{Z}^d)$, and will be denoted by $\mathcal{A}(\mathbb{Z}^d)$. Similarly, for other infinite subsets $\Lambda \subset \mathbb{Z}^d$ we define $\mathcal{A}(\Lambda)$ as the closure of the union of all $\mathcal{A}(\Lambda')$ with $\Lambda' \subset \Lambda$ finite.

When $x \in \mathbb{Z}^d$ is a lattice translation, we denote by $\tau_x$ the isomorphism from each $\mathcal{A}_y$ to $\mathcal{A}_{x+y}$, and its extension from $\mathcal{A}(\Lambda) \to \mathcal{A}(\Lambda+x)$, by shifting every site. Here we have used the notation $\Lambda+x = \{y+x|y \in \Lambda\}$ for shifted lattice subsets, which we also extend to $\Lambda_1+\Lambda_2 = \{x_1+x_2|x_1 \in \Lambda_1\}$.

A state $\omega$ of the spin system is a linear functional on $\mathcal{A}(\mathbb{Z}^d)$, which is positive in the sense that $\omega(1) = 1$. Equivalently, a state is given by a family $\omega_{\Lambda}$ of density operators on $(\mathbb{C}^d)^{\otimes \Lambda}$ (for each finite $\Lambda$), such that $\omega(X) = tr(\omega_{\Lambda} X)$ for $X \in \mathcal{A}(\Lambda)$. The local density matrices have to satisfy the consistency condition that, for $\Lambda_1 \subset \Lambda_2$, $\omega_{\Lambda_2}$ is obtained from $\omega_{\Lambda_1}$ by tracing out all tensor factors in $\Lambda_2 \setminus \Lambda_1$. Note that a state does not correspond to a configuration of a classical automaton, but rather to a probability distribution over global configurations.

**Definition 1** A Quantum Cellular Automaton with neighborhood scheme $\mathcal{N} \subset \mathbb{Z}^d$ is an homomorphism $T : \mathcal{A}(\mathbb{Z}^d) \to \mathcal{A}(\mathbb{Z}^d)$ of the quasi-local algebra, which commutes with lattice translations, and satisfies the locality condition $T(\mathcal{A}(\Lambda)) \subset \mathcal{A}(\Lambda+\mathcal{N})$ for every finite set $\Lambda \subset \mathbb{Z}^d$. The local transition rule of a cellular automaton is the homomorphism $T_0 : \mathcal{A}_0 \to \mathcal{A}(\mathcal{N})$.

Note that a unitary operator for the time evolution is not necessary in this formulation. Instead we have used it by its action on observables. Of course, the time step has to be read in the Heisenberg picture. That is, measuring some local observable $A \in \mathcal{A}(\Lambda)$ at time $t+1$ is equivalent to measuring the observable $T(A)$ at time $t$. The transition rule thus describes this backwards calculation for a single cell. $T_0(\mathcal{A}_0)$ is some isomorphic copy of the one-cell algebra embedded in a possibly quite complicated way into the algebra of neighboring cells. The relationship between the global evolution and the one-site transition rule is as simple as it should be:

**Lemma 2**

1. The global homomorphism $T$ is uniquely determined by the local transition rule $T_0$.
2. A homomorphism $T_0 : \mathcal{A}_0 \to \mathcal{A}(\mathcal{N})$ is the transition rule of a cellular automaton if and only if for all $x \in \mathbb{Z}^d$ such that $\mathcal{N} \cap (\mathcal{N}+x) \neq \emptyset$ the algebras $T_0(\mathcal{A}_0)$ and $\tau_x(T_0(\mathcal{A}_0))$ commute elementwise.

**Proof:** By translation invariance the action of $T_x : \mathcal{A}_x \to \mathcal{A}(\mathcal{N}+x)$ is determined as $T_x(A_x) = T_0 T_0 T_{x}^{-1}(A_x)$ on all other cells. Moreover, because $T$ is a homomorphism, the extension to any local algebra is also fixed. Explicitly, consider a product $\bigotimes_{x \in \Lambda} \mathcal{A}_x = \prod_{x \in \Lambda} \mathcal{A}_x$ of one-site operators. This equation just expresses our identification of the one site algebras $\mathcal{A}_x$ with subalgebras of $\mathcal{A}(\Lambda)$ by tensoring with unit operators. Then the homomorphism property of the global evolution requires that

$$T \left( \bigotimes_{x \in \Lambda} A_x \right) = \prod_{x \in \Lambda} T_x(A_x).$$

Note that the product on the right hand side cannot be replaced by a tensor product, because the factors have overlapping localization regions $x+\mathcal{N}$. Moreover, the argument of $T$ is a product of commuting factors, hence so is the right hand side. Hence the the commutativity condition (2) is necessary.

Conversely, if the factors $T_x(A_x)$ commute, their product is unambiguously defined. Since every local observable can be expressed as a linear combination of tensor products, Eq. (1) defines a homomorphism on the local algebra, as required. This shows the converse of (2), and since we have given an explicit formula of $T$ in terms of $T_0$ it also shows (1).

It is clear that the commutation condition of the Lemma can be expressed as a finite set of equations, and can therefore be verified effectively. Since only a small portion of the lattice is needed in this verification, the same steps are needed to check local transition rules for QCAs on graphs which locally look like $\mathbb{Z}^d$. Such graphs can be seen as integer lattices with periodic boundary conditions. The only condition we will need to impose is that the periods for the boundary condition are not too small compared with the size of neighborhood scheme $\mathcal{N}$ (a condition called “regularity” below). No algebraic conditions on the homomorphism $T_0$ are needed. Therefore we can turn the construction around, and immediately get a QCA on the infinite lattice from a QCA with finitely many cells. Since for finitely many cells a homomorphism is always just implemented by a unitary matrix, this allows us to define QCAs even for the infinite system, just by specifying unitary matrices with suitable properties.

Let us describe the periodic boundary QCAs more precisely and see what conditions are needed for the neighborhoods. The cells of a system with periodic boundary conditions arise from the cells in $\mathbb{Z}^d$ by identifying certain cells, namely all those differing by a vector $\gamma$ in some subgroup $\Gamma \subset \mathbb{Z}^d$. The set of cells is thus identified with the quotient $\mathcal{L} = \mathbb{Z}^d/\Gamma$. For each point in $x \in \mathcal{L}$, i.e., each equivalence class $x = x_0 + \gamma$, we can define the translation $x + n = x_0 + n + \gamma$. Consider now a neigh-
The neighborhood of \( x \in \mathcal{L} \) is then \( x + \mathcal{N} \subset \mathcal{L} \). Note that as far as the model with periodic boundary conditions is concerned we could change each \( n \in \mathcal{N} \) by a lattice vector in \( \Gamma \) without changing the neighborhood of any point. But since we are interested in the connection with the infinite model, we do not admit this ambiguity. The neighborhood scheme is called regular for the given periodic structure given by \( \mathcal{L} \), if the equations we have to check for the commutation rule of a cellular automaton are the same in both cases. Since these equations depend only on the intersections between translates of \( \mathcal{N} \) we only need to make sure that the geometry of intersections is the same. So suppose that neighborhoods on \( \mathcal{L} \) intersect, say \((x + \mathcal{N}) \cap (y + \mathcal{N}) \neq \emptyset \). This means that there is a translation \( m \in \mathbb{Z}^s \) such that \( x + m = y \) and also \( \mathcal{N} \cap (m + \mathcal{N}) \neq \emptyset \). Clearly, the first condition determines \( m \) up to a lattice translation \( \Gamma \), and the second is an intersection condition on the infinite lattice. Obviously, \((x + (\mathcal{N} \cap (N + m)) \subset (x + \mathcal{N}) \cap (y + \mathcal{N}) \). But the inclusion could be strict if there is more than one \( m \) with the required properties. This is precisely the case regularity must exclude. To summarize, we call a neighborhood scheme \( \mathcal{N} \subset \mathbb{Z}^s \) regular for a subgroup \( \Gamma \subset \mathbb{Z}^s \), if \( \mathcal{N} \cap (m + \mathcal{N}) \neq \emptyset \) and \( n \in \Gamma, n \neq 0 \), imply that \( \mathcal{N} \cap (m + n + \mathcal{N}) = \emptyset \). A more equivalent form is \((\mathcal{N} + \mathcal{N} - \mathcal{N} - \mathcal{N}) \cap \Gamma = \{0\}\). An example of a regular neighborhood is given in Figure 1. That the same neighborhood becomes non-regular for a smaller lattice is shown in Fig. 2.

![Periodic boundary conditions. The parallelogram represents the given finite lattice \( \mathcal{L} \), where cells cut by opposite boundaries must be suitably joined. The marks on the corners join up to a full circle. Two translates of the same neighborhood are shown. It is regular, because the geometry of intersections is the same as on the infinite plane.](image)

*FIG. 1:* Periodic boundary conditions. The parallelogram represents the given finite lattice \( \mathcal{L} \), where cells cut by opposite boundaries must be suitably joined. The marks on the corners join up to a full circle. Two translates of the same neighborhood are shown. It is regular, because the geometry of intersections is the same as on the infinite plane.

Then checking condition (2) of the Lemma for the QCA on \( \mathcal{L} \) and for the QCA on \( \mathbb{Z}^s \) are exactly equivalent. We call this useful principle the Wrapping Lemma:

**Lemma 3** The QCA transition rules on a finite lattice \( \mathcal{L} \) with respect to a regular neighborhood scheme \( \mathcal{N} \) are in one-to-one correspondence with the transition rules for QCAs on \( \mathbb{Z}^s \) with the same neighborhood scheme.

![The same neighborhood scheme is not regular on a 5x4 torus: Again we have two translates, but their intersection (cross-hatched) cannot be realized on the infinite square lattice as intersection of two such neighborhoods.](image)

*FIG. 2:* The same neighborhood scheme is not regular on a 5x4 torus: Again we have two translates, but their intersection (cross-hatched) cannot be realized on the infinite square lattice as intersection of two such neighborhoods.

### III. Basic Construction Methods

#### A. Commuting Unitaries and Phases

Consider a unitary operator \( U_0 \) in some local algebra \( \mathcal{A}(\mathcal{N}) \), which commutes with all its translates \( U_x = \tau_x(U_0) \), up to a phase. That is, we require that there are complex numbers \( \zeta_x \), with \( |\zeta_x| = 1 \) such that \( U_0 \tau_x(U_0) = \zeta_x \tau_x(U_0) U_0 \) for \((\mathcal{N} + x) \cap \mathcal{N} \neq \emptyset \). This is equivalent to

\[
U_x U_y = \zeta_{y-x} U_y U_x \tag{2}
\]

We can then formally define a unitary operator

\[
\" U = \prod_{x \in \mathcal{N}} U_x \" . \tag{3}
\]

Here the the scare quotes indicate that there is no way this infinite product can be made sense of. However, we can define instead the action of this “operator” on local observables. To this end, note that the actions \( A \mapsto U_x^* A U_x \) commute for different \( x \). Moreover, if \( x + \mathcal{N} \) does not intersect the localization region of \( A \), this action is the identity. Therefore, in the infinite product of these operations only a finite set is not the identity, and their product defines an automorphism \( T \). More formally, we have

\[
T(A) = \lim_{\Lambda \to \mathbb{Z}^s} U_\Lambda^* A U_\Lambda , \tag{4}
\]

where \( A \in \mathcal{A}(\mathbb{Z}^s) \), and \( U_\Lambda = \prod_{x \in \Lambda} U_x \). The limit is over any sequence of finite sets, eventually absorbing all lattice points, and if \( A \) is localized in a finite region, the limit is actually constant for sufficiently large \( \Lambda \).

The local transition rule is found by applying \( T \) to a single cell. This gives the neighborhood scheme

\[
\mathcal{N} = \bigcup_x (\mathcal{N} + x) \subset \mathcal{N} = \mathcal{N} - \mathcal{N} . \tag{5}
\]

We mention three special cases of this construction:

- When \( \mathcal{N} = \mathcal{N} = \{0\} \), we have to choose a unitary operator \( U_0 \in \mathcal{A}_0 \) acting on a single cell. Thus the cellular automaton acts by applying the same unitary rotation separately to every cell.
that have the strange property that they show unitaries, each of which appears in some local algebra $A(N)$ for some regular neighborhood $N$. Then the QCA is also well-defined on the infinite lattice.

However, this argument must be more subtle than it looks: it is well known, that the injectivity of a classical CA on the infinite lattice implies the existence of an inverse CA \[13\], but the inverse is hard to compute, because there is no a priori upper bound on its neighborhood size. Superficially, the inverse neighborhoods do not seem to enter the above argument. However, the argument for the locality $U^*AU \in A(N)$ requires more than the locality of the classical rule and the unitarity of $U$. Consider, for example, the rule
\[
c_{x+1}^t = c_x^t + c_{x-1}^t ,
\]
where $c_x^t \in \{0,1\}$, and addition is mod2. With periodic boundary conditions of length $L$ this is an invertible transformation unless $L$ is divisible by 3. This proviso is not of the form “for sufficiently large $L$...”, which means that the classical automaton does not allow a local inversion, i.e., there is no inverse cellular automaton. By the wrapping Lemma, it is clear that for this rule we cannot find a quantum version either\[19\]. This shows that the local invertibility of the classical CA must enter the argument. We therefore assume now that the classical CA is locally invertible, and the lattice $L$ is chosen sufficiently large, so that the neighborhood schemes for both the classical automaton and its inverse are regular for $L$.

The classical configurations are functions $a : L \rightarrow A$, where $A = \{1, \ldots, d\}$ denotes the set of classical states for each cell, and at the same time labels the computational basis of $\mathbb{C}^d$. We will write $a \in A^L$, and denote by $a_x$ the value of the cell $x$ in configuration $a$.

Extending this to a product basis, each configuration $a \in A^L$ determines a basis vector $|a\rangle$. Then the global unitary transition operator is defined by $U(a) = |F(a)\rangle$, where $F$ denotes the global classical transition function. The transition rule of the QCA is determined by computing all matrix elements of the operator $T_0(|c_0\rangle\langle c_0|)$, i.e.,
\[
\langle a|T_0(|c_0\rangle\langle c_0|)b\rangle = \langle a|U^*|c_0\rangle\langle c_0| \otimes I^{C\setminus \{0\}}U|b\rangle
= \langle F(a)|(|c_0\rangle\langle c_0| \otimes I^{C\setminus \{0\}})|F(b)\rangle
\]

This expression is $1 = 1$, if
\[
F(a)_0 = c_0, \quad \text{ and } F(a)_x = F(b)_x \quad \text{for } x \neq 0
\]
and $0 = 0$ otherwise. We have to show that this is of the form $X \otimes I^{\otimes C \setminus N}$.

**Lemma 4** Let $F$ be a classical cellular automaton with neighborhood scheme $N_C$, which has an inverse automaton with neighborhood scheme $N_I$. Then $T$ as defined above is a QCA with neighborhood scheme $N = N_C - N_C - N_I$. 

\[\quad\]
Of course, this Lemma only gives an upper bound on the size of the neighborhood scheme. Depending on the particular automaton, $N$ may be much smaller.

**Proof:** We have to show that for all $c_0, c_0$, the operator $T_0(|c_0\rangle\langle c_0|)$ is of the form $X \otimes 1 \otimes C_{\mathcal{N}}$ with $X \in \mathcal{A}(\mathcal{N})$. This is equivalent to two conditions: on the one hand the matrix elements $(a|T_0(|c_0\rangle\langle c_0|)|b\rangle) = 0$ must vanish, whenever $a_x \neq b_x$ for some point $x \notin \mathcal{N}$, and, moreover, the value of the matrix elements must be independent of $a_x$ for such $x$.

Suppose that the matrix element is non-zero, i.e., condition $\mathbf{8}$ holds. Then for all $y$ such that $y + N_I \neq 0$ the computation of the the values of $a_y$ and $b_y$ from $F(a)$ and $F(b)$ will give the same values of $a_y$ and $b_y$. In other words, the diagonality condition holds for $y \notin (-N_I)$.

The dependence of the matrix element on $a_x$ is also governed by condition $\mathbf{8}$: since the matrix elements can only be 0 or 1, we have to show that the validity of the condition does not depend on $a_x$ for $x \notin \mathcal{N}$, given the range of equality of $a$'s and $b$'s established in the previous paragraph. Indeed, once that diagonality is established, one can see that most of the conditions $\mathbf{8}$ become redundant. If $x$ is such that $(x + N_C) \cap (-N_I) = \emptyset$, then $F(a)_x$ and $F(b)_x$ are computed by the local rule of $F$ from identical data, so they must be equal. It therefore suffices to consider the condition for those finitely many $x$ for which a dependence remains possible, i.e., $x \in (-N_C - N_I)$. But then only those $a_x$ enter, which contribute to $F(a)_x$ via the local rule (and similarly for $b$). This restricts $y$ to $(N_C - N_C - N_I)$, and this is what the Lemma claims as the localization region. \hfill \Box

### C. Partitioning

The easiest way to build a cellular automaton with readily verified locality properties is based on the cellwise unitary rotations, with the modification of changing the partitioning of the system into cells [20]. The typical construction would thus be:

1. possibly divide the given cells into suitable subcells, by writing the one-cell Hilbert space $C_d$ as a tensor product of other spaces.

2. partition the set of cells of the previous step into blocks in some periodic way: every cell now belongs to exactly one block, and any two blocks are connected by a lattice translation.

3. apply the same unitary operator to each block algebra.

4. possibly repeat this procedure with different block partitions

5. possibly split and regroup once again to come back to the original pattern of $d$-dimensional cells.

Every step in this construction is well-defined for the global system for the same reason that cell-wise rotations are valid QCA operations. Moreover, the unitary operators doing each of the steps are essentially arbitrary, and by just inverting the steps we can immediately construct the inverse QCA. This is why partitioned cellular automata are sometimes called **structurally reversible**. Moreover, the partitioning idea allows one to construct QCAs from irreversible local rules just as easily as reversible ones [10, 14].

Our main theorem (Theorem 6 below) will tell us that every QCA can be written in partitioned form. For nearest neighbor automata it is sufficient to take two steps in which cells are grouped in cubes of side 2, possibly with a choice of unequal cell sizes in the intermediate step (see Section IV A). This is known as the Margolus partitioning scheme (see Figure 3).

**FIG. 3:** The Margolus partitioning scheme in $s = 2$ dimensions. Operations are alternatingly applied to the solid and to the dashed partitioning into $2 \times 2$ squares. The square shape of the cells is irrelevant, as they only serve to label localized quantum systems.

### D. Circuits

Of course, it is natural to think of a cellular automaton as a physical device, which just happens to be infinitely extended (or periodically closed). This suggests building QCAs from some basic supply of circuit elements, whose properties will then ensure that the overall operation makes sense. The mathematical details of the description must then work out automatically, because “Hardware cannot lie”. Consider the following example

**FIG. 4:** A proposed QCA circuit.

Here the flow of information is from top to bottom.
The symbol stands for a CNOT gate, by which the bit on the line with circle and cross (the “target bit”) is flipped if and only if the value of the bit on the line with the fat dot (the “control bit”) is “1”. This is a standard gate also for quantum computation. We can readily compute the action of this device on classical information: each output bit depends only on the input on the same line and the line one step to the right. Presumably, this would also be the description of the action on computational basis states in the quantum case. So can we not just build this device, and construct its proper mathematical description along with the hardware?

The problem with this automaton becomes apparent already when we try to compute its classical inverse: this requires at each switch to know the value of a control bit, which is not yet determined. In fact, the inverse does not exist, because the initial states “all 1” and “all 0” are both mapped to “all 0”. So this device is not reversible, even classically. (Incidentally, this also holds for periodic boundary conditions, so it is not a problem of infinite size). What went wrong? The problem is the timing of the gates. In fact, in the usual gate model of quantum computation it is assumed that each gate is executed at a certain time. Here the times overlap, and if we insist on the gates being executed, say from the left to the right, we either need infinitely many operation times per step, or we run into time ordering problems at the boundary condition.

One way to avoid this problem is to insist on some finite number of clock cycles per QCA step, that each gate is executed in one of these cycles, and that the gates running in the same cycle do not access the same registers. An “unscrambled version” of the above impossible QCA is drawn in Fig. 5.

FIG. 5: An operational QCA circuit taking two clock cycles

Clearly, this is a partitioning QCA and, in fact, the description we just gave of a circuit with timing constraints is nothing but the definition of a partitioning QCA.

E. Clifford automata

In the implementation of quantum computation there is often a separation between “easily implemented” operations and others, which may be more costly. For example, ”linear” transformations on the quantum light field can be performed with mirrors, beam splitters and phase plates, whereas squeezing or photon number counting are more costly. A similar choice of a subgroup of “easy” operations for qubit quantum computation is the group of transformations, which take tensor products of Pauli matrices into tensor products of Pauli matrices, the so-called Clifford group. Indeed in some implementations these play a special role, and can be executed in parallel. Clearly, it is important to understand this subgroup completely, although it is also clear that such transformations alone will not allow quantum computational speedup.

The natural mathematical setting for the investigation of Clifford QCAs are discrete Weyl systems, with a finite Weyl system acting at each site, and the tensor products of one-site Weyl operators generating a Weyl system with infinitely many degrees of freedom. If the local Weyl system has prime dimension, one can give a very explicit description of the group of Clifford QCAs, which will be presented elsewhere. For illustration let us just take qubit automata $d = 2$ in one dimension.

What is needed to define such an automaton? Since the Pauli matrices $\sigma_x$ and $\sigma_z$ generate the one site algebra, we only need to specify the two operators $T_0(\sigma_x)$ and $T_0(\sigma_y)$. The Clifford property means that these two operators must be tensor products of Pauli matrices, so we have

\[
T_0(\sigma_x) = \sigma_{\xi-N} \otimes \cdots \sigma_{\xi_0} \otimes \cdots \sigma_{\xi_N} = \sigma(\xi)
\]

\[
T_0(\sigma_z) = \sigma_{\eta-N} \otimes \cdots \sigma_{\eta_0} \otimes \cdots \sigma_{\eta_N} = \sigma(\eta),
\]

where each $\xi$, $\eta$ can take the values $0, x, y, z$, with $\sigma_0 = 1$. Now the two strings $\xi = (\xi_{-N}, \ldots, \xi_N)$ and $\eta = (\eta_{-N}, \ldots, \eta_N)$ completely characterize the automaton. But which strings are allowed? From the general theory we immediately get the necessary and sufficient conditions: $\sigma(\xi)$ must commute with all its translates, the same holds for $\sigma(\eta)$. Moreover, $\sigma(\xi)$ commutes with $\tau_i(\sigma(\eta))$ for $i \neq 0$ and anti-commutes for $i = 0$. Since tensor products of Pauli matrices always either commute or anti-commute, one can run a computer search for all examples with low neighborhood size $N$. This turns up the surprising result that (up to a common translation) the strings $\xi$ and $\eta$ must be palindromes, i.e., $\xi_{-k} = \xi_k$.

The general theory confirms this, and moreover establishes an isomorphism of the group of Clifford QCAs with the group of $2 \times 2$-matrices,

\[
\begin{pmatrix}
\xi_+(z) & \eta_+(z) \\
\xi_-(z) & \eta_-(z)
\end{pmatrix},
\]

whose entries are polynomials over the two-element field $F_2 = \{0, 1\}$ in one indeterminate $z$, such that the determinant is the constant polynomial 1. Here the coefficients of $\xi_k$ are bit strings which together determine the string $\xi_0, \xi_1, \ldots, \xi_N$ used in Eq. 9.

One can also find a simple set of generators: Apart from one-site transformations and the shift only one QCA is needed:

\[
T_0(\sigma_x) = 1 \otimes \sigma_x \otimes 1
\]

\[
T_0(\sigma_z) = \sigma_x \otimes \sigma_x \otimes \sigma_x,
\]

possibly, however, acting not between neighboring sites as written here, but between sites at a fixed distance $L$, so that the chain breaks up into $L$ non-interacting chains.
The prototype \( \mathbf{11} \) has a number of interesting properties. For example, the iterates \( T^n(\sigma(z)) \) of an initial Pauli product \( \sigma(z) \) have a specific form: they consist of a Pauli product moving to the left, and another one moving to the right, each at maximal speed, and the expanding space between these patterns is filled by one of four possibilities: all \( \mathbf{1} \), all \( \sigma_y \) or an alternating patterns of \( \sigma_x \otimes \sigma_y \), or the same shifted by one cell.

### IV. STRUCTURE

In this section we will employ the commutativity property of transition rules to get some information about the structure of possible rules, aiming at the proof that all QCA transition rules can be understood in a partitioning scheme.

Without loss of generality, we consider only nearest neighbor rules on a cubic lattice. For a non-cubic lattice we can choose a family of basic cells (a “fundamental domain”) such that all cells are generated from these basic ones by translation symmetries. By considering the fundamental domain and its translates as new cells, we effectively get a family of lattice cells labelled by \( \mathbb{Z}^s \). If the neighborhood scheme involves more than nearest neighbors, we can again enlarge cells. Of course, these operations partly destroy the underlying lattice symmetry, so that operations on regrouped cells may fail to have the translation (or other) symmetry of the original lattice. However, for the proof of structural invertibility a regrouped lattice of “supercells” works just as well.

We begin by describing the geometry of the generalized Margolus partitioning scheme. In the following subsection we state the main theorem: this scheme indeed suffices for all QCAs. The proof relies on the concept of “support algebras”, and is described in Subsection IV.C. When the support algebras are abelian, one can characterize the possible QCAs at the single cell level, without partitioning (see Subsection IV.E). This allows us to determine explicitly all nearest neighbor qubit automata in one dimension (Section IV.G).

#### A. Generalized Margolus Partitioning

Consider a cellular automaton with one-site algebra \( \mathcal{A}_0 = \mathcal{M}_d \), lattice \( \mathbb{Z}^s \), and nearest neighborhood scheme:

\[
\mathcal{N} = \{ x \in \mathbb{Z}^s \mid \forall_i |x_i| \leq 1 \} .
\]

We will use a cell grouping introduced by Margolus \( \mathbb{Z}^2 \). In this scheme one “supercell” is the unit cube

\[
\square = \{ x \in \mathbb{Z}^s \mid \forall_i x_i = 0, 1 \} ,
\]

which consists of \( 2^s \) cells. The even translates \( \square + 2x \) with \( x \in \mathbb{Z}^s \) cover the whole lattice. We denote by \( Q \) the set of \( 2^s \) quadrant vectors \( q \in \mathbb{Z}^s \) for which each component is \( q_i \in \{-1,+1\} \) (see Fig. 6). In particular the vector into the positive quadrant (with all \( q_i = +1 \)) will be denoted by \( \mathbf{1} \). Note that the sum of two quadrant vectors is an even lattice translation in \( 2\mathbb{Z}^s \). Moreover, the \( 2^s \) cubes \( \square + q \) for \( q \in Q \) are disjoint and their union contains all neighborhoods of cells in \( \square \). Just like the even translates of \( \square \), the cubes \( \square + 1 + 2x \) with \( x \in \mathbb{Z}^s \) form a partition of the lattice (compare Fig. 6).

A partitioned automaton based on the Margolus scheme would alternatingly apply blockwise unitary transformations to the cubes in the two partitions. But not every QCA can be written in this way. A good counterexample is the shift in the quadrant direction \( \mathbf{1} \). Here the entire quantum information in the \( \mathbb{Z}^s \) cells \( \square \) will have to be moved to \( \square + \mathbf{1} \) although these blocks have only a single cell as overlap. It turns out, however, that a slight generalization of the Margolus scheme suffices to represent every QCA: all we have to do is to allow different cell sizes in the intermediate step. For the rest of this subsection we will explain the resulting scheme.

With each quadrant vector \( q \in Q \) we associate an observable algebra \( \mathcal{B}_q \subset \mathcal{A}((\square + q)) \), which is isomorphic to the algebra of \( n(q) \times n(q) \)-matrices for some integer \( n(q) \). Since \( \mathcal{B}_q \) is contained in a local algebra, it makes sense to consider its (even) translates \( \tau_x(\mathcal{B}_q) \subset \mathcal{A}((\square + q + x)) \) with \( x \in 2\mathbb{Z}^s \). In particular, \( \mathcal{A}((\square + 1)) \) contains all the algebras \( \tau_{-q}(\mathcal{B}_q) \). A crucial assumption of our construction is that these subalgebras of \( \mathcal{A}((\square + 1)) \) commute, and together span \( \mathcal{A}((\square + q)) \). This is possible if and only if the equation

\[
\prod_{q \in Q} n(q) = d^{2^s}
\]

holds for the matrix dimensions. Note that each cell \( \mathcal{A}((\square + x)) \) has this dimension, whether or not \( x \) is even or not.

The local rule of an automaton now defines (and is
defined by) a homomorphism
\[ T_\square : \mathcal{A}(\square) \to \prod_{q \in Q} \mathcal{B}_q. \tag{15} \]

Since the dimensions of domain and range are the same, such a homomorphism is necessarily an isomorphism, i.e., we can find suitable bases in each cell and for each of the matrix algebras \( \mathcal{B}_q \) such that \( T_\square(A) = UAU^* \) for a unitary operator
\[ U : \bigotimes_{x \in \square} \mathbb{C}^d \to \bigotimes_{q \in \mathbb{Q}} \mathbb{C}^{n(q)}. \tag{16} \]

Such a unitary operator by itself does not fix a QCA, because if we only take \( \mathcal{B}_q \) as an abstract matrix algebra, we still need to specify how \( \tau_{1-q} \mathcal{B}_q \) is contained in \( \mathcal{A}(\square + 1) \) or, equivalently, to specify the isomorphism of \( \bigotimes_q \tau_{1-q} \mathcal{B}_q \) with \( \mathcal{A}(\square + 1) \). This will be affected by another unitary operator
\[ V : \bigotimes_q \mathbb{C}^{n(q)} \to \bigotimes_q \mathbb{C}^d. \tag{17} \]

Any pair of unitaries \((U, V)\) according to Eqs. \((16,17)\) specifies a transformation \( T \) on local algebras, which satisfies all requirements for a cellular automaton, except translation invariance: \( T \) only commutes with even translations. The scheme in one and two lattice dimensions is visualized in Figures 7–9.

**FIG. 7:** Generalized Margolus Scheme in \( s = 1 \) dimension. The algebras \( \mathcal{B}_{+1} \) and \( \mathcal{B}_{-1} \) are symbolized by the different size cells in the intermediate step.

If we want \( T \), as constructed from unitaries \( U \) and \( V \), to be a proper cellular automaton with full translation invariance, there will be additional conditions on these unitaries. Unfortunately, these conditions are not easily written down and solved in the general case. We also note that \( U \) and \( V \) are not uniquely determined by the automaton: we have the freedom to choose a basis in every \( \mathbb{C}^{n(q)} \). Changing this basis amounts to a cellwise rotation included in \( U \), which is immediately undone by the \( V \)-step. The key feature of automata in a partitioned scheme is structural reversibility, as described in the following Lemma.

**Lemma 5** Let \( T \) be a homomorphism constructed from unitaries \( (U, V) \) in the generalized Margolus scheme. Then \( T \) is invertible, and \( T^{-1} \) is also a generalized Margolus automaton. Moreover, if \( T \) commutes with all (not just even) translations, then both \( T \) and \( T^{-1} \) are nearest neighbor QCA.s.

Proof: The Margolus unitaries defining \( T^{-1} \) are \((V^*, U^*)\). To check the localization properties, it is helpful not to think of these transformations in the apparently time-asymmetric scheme of Fig. 5 but to take \( \mathcal{B}_q \) as an algebra localized in the intersection of the cubes \( \square \) and \( (\square + q) \), i.e., as localized at the cell \((1+q)/2\). Note that \( T^{-1} \) is a two-sided inverse, and hence uniquely determined by \( T \).

Therefore, if \( T \) commutes with all translations, so does \( T^{-1} \). It remains to check that if \( T \) is a Margolus automaton commuting with translations, it is actually a nearest neighbor automaton, i.e., a QCA with neighborhood scheme \( \mathcal{N} \) from \((12)\). Since, for every \( x \in \square \), we have \( 0 \in (\square - x) \), we have
\[ T(\mathcal{A}_0) \subset T(\mathcal{A}(\square - x)) \subset \bigotimes_{q \in Q} \mathcal{A}(\square + q - x). \tag{18} \]

Since this is valid for all \( x \in \square \), we have \( T(\mathcal{A}_0) \subset \mathcal{A}(\mathcal{N}) \), with
\[ \mathcal{N} = \bigcap_{x \in \square} \bigcup_{q \in Q} (\square + q - x) = \mathcal{N}. \tag{19} \]
B. Main Theorem

Theorem 6 Let $T$ be the global transition homomorphism of a nearest neighbor quantum cellular automaton on the lattice $\mathbb{Z}^d$ with single-cell algebra $A_0 = M_d$. Then $T$ can be represented in the generalized Margolus partitioning scheme, i.e., $T$ restricts to an isomorphism

$$T : \mathcal{A}(\square) \rightarrow \bigotimes_{q \in Q} \mathcal{B}_q,$$  

(20)

where for each quadrant vector $q \in Q$, the subalgebra $\mathcal{B}_q \subset \mathcal{A}(\square + q)$ is a full matrix algebra, $\mathcal{B}_q \cong M_{n(q)}$. These algebras and the matrix dimensions $n(q)$, which satisfy Eq. (14), are uniquely determined by $T$.

Combining this with Lemma 3 we get

Corollary 7 The inverse of a nearest neighbor QCA exists, and is a nearest neighbor QCA.

Note that this result is in stark contrast to the classical situation. In the classical case the inverse of an injective CA is a CA, i.e., locally invertible, but it is a highly non-trivial matter to determine the neighborhood scheme of the inverse, which can be much larger than the neighborhood of the automaton itself. This is not a contradiction with the observation that every classical CA can be quantized (see Section III B): In order to construct a QCA from a classical CA, we needed the neighborhood size of the inverse.

The proof of the Theorem will be given in subsection IV D. The key idea is to construct $\mathcal{B}_q \subset \mathcal{A}(\square + q)$ explicitly from the inclusion $T(\mathcal{A}(\square)) \subset \bigotimes_{q} \mathcal{A}(\square + q)$. This construction, which will also be useful independently, will be described in the next section.

C. Support Algebras of Local Rules

By definition, the transition rule $T_0$ maps one cell algebra into a tensor product of neighboring ones. Therefore we need to investigate just how one subalgebra can sit inside a tensor product of others.

Consider a subalgebra $A \subset B_1 \otimes B_2$ of tensor product. For the moment let us forget about the multiplication laws, and just consider these as vector spaces, with the tensor product known from the (multi-)linear algebra of finite dimensional vector spaces. Then we can expand each $a \in A$ into a sum $a = \sum_{\mu} b_{\mu}^{(1)} \otimes b_{\mu}^{(2)}$. But we might get by just using a small subset of operators $b_{\mu}^{(i)}$. The smallest subspace of $B_1$ sufficient for these expansions will be called the support of $A$ on the first factor, and will be denoted by $s(A, B_1)$. For a more formal definition note that each $a \in A$ can be expanded uniquely in the form $a = \sum_{\mu} a_{\mu} \otimes e_{\mu}$, where $\{e_{\mu}\}$ is a fixed basis of $B_2$. Then $s(A, B_1)$ is the linear span of all $a_{\mu}$ in this expansion, and is clearly independent of the basis $\{e_{\mu}\}$ chosen for $B_2$. Then it is clear that $b_{\mu}^{(i)} \in s(A, B_i)$ indeed suffice to expand every $a \in A$, i.e.,

$$A \subset s(A, B_1) \otimes s(A, B_2) \subset B_1 \otimes B_2.$$  

(21)

The analogous relation for $A$ contained in a tensor product of more factors is seen in the same way.

Now we remember the algebraic structure: $s(A, B_1)$ is a linear subspace of a C*-algebra, so we can define the support algebra $S(A, B_1)$ of $A \subset \bigotimes_{i} B_i$ on one factor $B_i$ as the subalgebra of $B_i$ generated by the elements of $s(A, B_i)$. Then we also have

$$A \subset S(A, B_1) \otimes S(A, B_2) \subset B_1 \otimes B_2.$$  

(22)

Note that since any observable algebra $A$ is closed under adjoints, so is $S(A, B_1)$. The crucial fact we need about such inclusions is the following:

Lemma 8 Let $A_1 \subset B_1 \otimes B_2$ and $A_2 \subset B_2 \otimes B_3$ be subalgebras such that $A_1 \otimes 1_3$ and $1_1 \otimes A_2$ commute in $B_1 \otimes B_2 \otimes B_3$. Then $S(A_1, B_2)$ and $S(A_2, B_2)$ commute in $B_2$.

Proof. Pick bases $\{e_{\mu}\} \subset B_1$ and $\{e'_{\nu}\} \subset B_2$, and let $a \in A_1$ and $a' \in A_2$. Then we may expand uniquely:

$$a = \sum_{\mu} e_{\mu} \otimes a_{\mu} \quad \text{and} \quad a' = \sum_{\nu} e'_{\nu} \otimes a'_{\nu}.$$  

Then by assumption

$$0 = [a \otimes 1_3, 1_1 \otimes a'] = \sum_{\mu \nu} e_{\mu} \otimes [a_{\mu}, a'_{\nu}] \otimes e'_{\nu}.$$  

Now since the elements $e_{\mu} \otimes e'_{\nu}$ are a basis of $B_1 \otimes B_3$, this expansion is unique, so we must have $[a_{\mu}, a'_{\nu}] = 0$ for all $\mu, \nu$. Clearly, this property also transfers to the algebras generated by the $a_{\mu}$ and $a'_{\nu}$, i.e., to the support algebras noted in the Lemma.

D. Proof of the Main Theorem

We apply the construction of support algebras to the inclusion

$$T(\mathcal{A}(\square)) \subset \bigotimes_{q} \mathcal{A}(\square + q)$$  

(23)

and define

$$\mathcal{B}_q = S(T(\mathcal{A}(\square)), \mathcal{A}(\square + q)).$$  

(24)

As a finite dimensional C*-algebra, each $\mathcal{B}_q$ is isomorphic to $\mathcal{B}_q = \bigoplus_{\mu} M_{n(q, \mu)}$. (See Proposition 11.) Now $T(\mathcal{A}(\square))$ is homomorphically embedded into $\bigotimes_{q} \mathcal{B}_q$, with $T(1) = 1$. Hence by Proposition 12 we know that for any
choice of summands $\mu_q$ we must have that $d^{2^s}$, the matrix dimension of $A_{D}$, divides $\prod_q n(q, \mu_q)$. This gives a lower bound on the block sizes.

In order to get an upper bound, consider the support algebras contained in some shifted cube, such as $D + 1$. These are

$$S(T(A(D + 1 - q)), A(D + 1)) = \tau_{1 - q} S(T(A(D)), A(D + q)) = \tau_{1 - q}(B_q)$$

Since the $A(D + 1 - q)$ commute, so do their images under $T$ and, by Lemma 8, so do the algebras $\tau_{1 - q}(B_q) \subset A(D + 1)$. However, we do not know a priori that these algebras are contained in $A(D + 1)$ as a tensor product.

When $z_{q, \mu_q} \in B_q$ is a central projection onto one of the matrix blocks of $B_q$, it is clear that the product $\prod_q z_{q, \mu_q}$ is a central element of the algebra generated by the $B_q$, but it might be zero. On the other hand, there must be some choice of blocks $\mu_q$, for which this is non-zero, and for this combination $\prod_q M_{n(q, \mu_q)}$, which is isomorphic to $\mathcal{M}_n$ with $n = \prod_q n(q, \mu_q)$, is a direct summand of $\prod_q B_q \subset A(D + 1)$. Hence we get the inequality

$$d^{2^s} \geq \prod_q n(q, \mu_q).$$

On the other hand, by the first step, the left hand side divides the right hand side of this inequality, so the we must have equality. This also implies that only one summand can be present in $B_q$, so we get $B_q \cong M_{n(q)}$ with $n(q) = n(q, \mu_q)$. That $T$ is an isomorphism from $A(D)$ onto $\otimes_q B_q$ follows by a direct dimension count, since a $*$-homomorphism between full matrix algebras of equal dimension can only be zero or an isomorphism.

E. QCAs with abelian neighborhood

In a sense, Theorem 8 gives a complete constructive procedure for QCAs in terms of the two unitary operators $U, V$ with a constraint. Unfortunately, however, it does not seem to be easy to give a general solution of the constraint equations expressing the translation invariance (rather than the invariance by even translations). Therefore it is suggestive to repeat the analysis of support algebras also on the single cell level. Setting

$$D_x = S(T_0(A_0), A_x)$$

we have

$$T_0(A_0) \subset \bigotimes_{x \in \mathcal{N}} D_x$$

It is clear that since $T_0(A_0)$ is non-abelian, at least one of the algebras $D_x$ must also be non-abelian. The simplest case in this regard will be when all $D_x$ are abelian and commute with each other, except one, say $D_0$, which then has to isomorphic to the full cell algebra $A_0$ by Property 12. Since all $D_x$ commute, we can jointly diagonalize them and this fixes a canonical basis for every cell. When $|\mu\rangle$ denotes the basis vectors, we can write the local transition rule as

$$T_0(A) = \sum_{\mu, \nu} |\mu\rangle \langle \mu| \otimes |\nu\rangle \langle \nu| \otimes B_{\mu, \nu}$$

where the sum runs over all tuples $|\mu\rangle, |\nu\rangle$ of basis labels $|\mu\rangle$ for $x \in \mathcal{N}, x \neq 0$ and, for each such tuple, $U(|\mu\rangle)$ is a unitary operator. Thus $T_0$ describes a conditional unitary operation on cell 0, where the conditioning is in some fixed “computational basis”.

We now need to analyze the constraints on these unitaries needed to make this homomorphism $T_0$ a local transition rule. As a first step we look at the simplest case:

**Lemma 9** Let $U_{\mu}, V_{\nu} \in \mathcal{M}_d$ be unitary operators $(\mu, \nu = 1, \ldots, d)$ such that, for all $A, B \in \mathcal{M}_d$,

$$\sum_{\mu, \nu} \left[ U_{\mu}^* A U_{\mu} \otimes |\mu\rangle \langle \mu| \otimes V_{\nu}^* B V_{\nu} \right] = 0$$

Then there are unitary $U, V \in \mathcal{M}_d$ such that, for all $\mu, U^* U_{\mu}$ and $V^* V_{\mu}$ are diagonal.

**Proof.** Let us abbreviate $A_{\mu} = U_{\mu}^* A U_{\mu}, B_{\nu} = V_{\nu}^* B V_{\nu}$, and take the matrix element of equation (29) in the product basis vectors $\langle \alpha| \beta \cdots |\gamma\rangle$. This gives

$$\langle \alpha| \beta \cdots |\gamma\rangle \langle \beta| B_{\nu} |\delta\rangle = \langle \alpha| \beta \cdots |\gamma\rangle \langle \beta| B_{\nu} |\delta\rangle$$

Now set $B = V_{\alpha}^* |\beta'\rangle \langle \delta'| V_{\alpha}$, with $\beta' \neq \beta$. Then $B_{\nu} = |\beta'\rangle \langle \delta'|$, and $\langle \beta| B_{\nu} |\delta\rangle = 0$, and the right hand side vanishes. Hence, for every $A$ and every $\delta'$

$$\langle \alpha| \beta \cdots |\gamma\rangle \langle \beta| V_{\alpha}^* V_{\beta} |\beta'\rangle \langle \delta'| V_{\alpha}^* V_{\gamma} |\delta\rangle = 0.$$
Hence we can apply the Lemma to the commutator separately for every pair $\mu, \nu$, and we find that up to a common unitary all $U_{\mu \nu}$ have to commute. Again, up to a cell-wise unitary rotation, we can choose the common eigenbasis of the $U_{\mu \nu}$ as the same basis in which the conditions are written, i.e.,

$$U_{\mu \nu} = \sum_{\kappa} u(\mu \nu) |\kappa\rangle\langle \kappa| , \quad (33)$$

with some phase function $u$ depending on three neighboring basis labels. However, this phase function $u$ is not arbitrary: unitaries of the form $u$ in this way may still fail to satisfy (32). If we insert $A = |a\rangle\langle b|$ and $B = |a'\rangle\langle b'|$ we get the functional equation

$$\frac{u(\mu ba')}{u(\mu a^2)} \cdot \frac{u(bb' \nu')}{u(ba' \nu')} = \frac{u(\mu bb')}{u(\mu ab)} \cdot \frac{u(ab' \nu')}{u(aa' \nu')} . \quad (34)$$

Since we want to classify solutions up to a cell-wise rotation, we can take one of the unitaries $U_{\mu \nu}$ to be the identity, say $U_{11} = I$, or $u(1x) = 1$. Moreover, an overall phase of $U_{\mu \nu}$ is irrelevant, and we can choose this so $u(\mu 1\nu) = 1$. Then in (34) we take $a = b' = \nu' = 1$, which gives

$$u(\mu ba') = u(\mu b1)u(ba'1) \quad (35)$$

Thus $u$ is already determined by the two-variable function $(a, b) \mapsto u(a, b, 1)$. It is easy to check that any choice of this function yields a solution of (32) via (35).

We can summarize the result as follows:

**Proposition 10** Let $T_0$ be the local transition rule of a QCA such that $\mathcal{D}_1$ and $\mathcal{D}_{-1}$ are both abelian. Then, with respect to a basis in which these algebras are diagonal, there is a phase gate on $\mathbb{C}^d \otimes \mathbb{C}^d$:

$$U = \sum_{ab} u(a,b)|ab\rangle\langle ab| , \quad (36)$$

normalized such that $u(1,b)ab\rangle\langle ab|$, and a one-site unitary $V$ such that

$$T_0(A) = X^*(\mathbb{I} \otimes V^*AV \otimes \mathbb{I})X \quad \text{with} \quad X = (U \otimes I_3)(I_1 \otimes U) .$$

**F. Unilateral Automata**

Another case of automata in one dimension, which can be characterized completely, are automata with neighborhood scheme $\mathcal{N} = \{0, 1\}$ (or, symmetrically, $\mathcal{N} = \{-1, 0\}$). The analysis is almost identical to that of Theorem and gives full matrix algebras $\mathcal{D}_i = S(T_0(A_0), A_i) = \mathcal{M}_n$, and such that $n_0n_1 = d$. As in the case of the Theorem, the local rules combines an arbitrary unitary $U : \mathbb{C}^d \rightarrow \mathbb{C}^{n_0} \otimes \mathbb{C}^{n_1}$ with a unitary $V : \mathbb{C}^{n_1} \otimes \mathbb{C}^{n_2} \rightarrow \mathbb{C}^d$. We only mention these to state the following classification of the simplest case:

**G. Nearest neighbor qubit automata in one dimension**

Consider the right and left support algebras $\mathcal{D}_{-1}, \mathcal{D}_0, \mathcal{D}_{+1}$ as in (27). These are subalgebras of the $2 \times 2$-matrices, which leaves three possibilities: each of these algebras can either be trivial ($\mathcal{D}_1 = \mathbb{C} I$), an abelian two-state algebra (isomorphic to the diagonal matrices, or the full algebra $\mathcal{M}_2$.

Suppose that at least one of the algebras $\mathcal{D}_{\pm1}$, say $\mathcal{D}_{-1}$, is trivial. Then we have a unilateral automaton. Since $n_0n_1 = 2$ we must have either $n_0 = 2, n_1 = 1$, a cell-wise unitary rotation or $n_0 = 1, n_1 = 2$ a right shift, possibly combined with a cell-wise rotation.

Suppose that none of the algebras $\mathcal{D}_{\pm1}$ is trivial. Then because $\mathcal{D}_{-1}$ commutes with $\mathcal{D}_{+1}$ neither algebra can be the full matrix algebra, since that would force the other to be trivial. It follows that both are abelian, and commute. Hence after a basis change (by another cell-wise rotation) we can take $\mathcal{D}_{-1} = \mathcal{D}_{+1}$ as the algebra of diagonal $2 \times 2$-matrices. This brings us into the situation of Section IV-E, and we find a phase rotation. Choosing the normalization in Proposition 10 we have only one free parameter left, i.e., we have an automaton built from commuting unitaries $U_x$ (cf. Section III), which are phase gates

$$U_x = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix} . \quad (37)$$

The classification is hence complete. It is represented in Fig.10

![Fig. 10: All nearest neighbor qubit automata arise by combining cell-wise unitary rotations (C) with right shifts (R), left shifts (L), or phase gates (P).](image-url)

It is interesting to compare this with the classical case, which can be stated very similarly: then the only cell-wise operations are identity and global flip. Of course,
the possibility of phase gates does not arise, leaving 6 classical possibilities.

Beyond qubits, a good classification exists for Clifford automata in prime dimension. However, for general three-level systems the classification is likely to be complicated, since there is already a host of reversible classical nearest neighbor automata.

V. OTHER APPROACHES

In this section we take a look at the various proposals for defining QCAs, and show how they relate to the approach taken in this paper.

A. Feynman, and Transition Quasi-Probabilities

The idea of a quantum cellular automaton is clearly present in Feynman’s famous 1981 lecture. Although he suggests not only that a theory might and should be developed, and that it might even be taken seriously as fundamental physical theory, he does not actually develop a notion of QCAs in this article. The context in which he does write down a transition rule for a QCA, is where he discusses the possibility of simulating a QCA with a probabilistic cellular automaton. He emphasizes that this would involve something like negative transition probabilities and closes this section saying “... I wanted to explain that if I try my best to make the equations look as near as possible to what would be imitable by a classical probabilistic computer, I get into trouble”.

Feynman’s idea for making a QCA look as classical as possible is to replace “transition probabilities” by Wigner function-like “transition quasi-probabilities”. This approach is an interesting contribution to the definition of irreversible QCAs, which is still plagued with problems. However, as Feynman is clearly aware, it fails, and it is instructive to analyze this failure in the case of reversible automata.

The transition function of a classical probabilistic cellular automaton (for a set $S$ of single-cell states) is a set of probabilities $M(s′|s_N)$ specifying the probability of finding a state $s′ \in S$, when the configuration of the neighbors at the previous time step is $s_N$. Using the “simultaneous and independent update rule” the probability for finding a configuration $s_A$ in a finite region $A \subset \mathbb{Z}^d$ becomes

$$M(s_A′|s) = \prod_{x \in A} M(s_A′|s_{N+|x|}). \tag{38}$$

Note that this is readily read as a statement in the Heisenberg picture: the probability for $s_A′$ is expressed as the expectation of a random variable in the previous time step, namely the right hand side of $M(s′|s_N)$, considered as a function of the variables $s_x$. In the quantum case, $M(s′|s_N)$ would then become an observable in $A_N$, depending in a linear (and completely positive) way on an observable $s′ \in A_0$. This is precisely a description of the local transition rule $T_0$. Note that the commutation condition for local rules (Lemma 2) implies that the product is well-defined, independently of the ordering of the factors. In a more general quantum context, such as irreversible QCA evolutions for which the global rule will not respect the product, we cannot be sure of this property: additional information about the ordering of factors in $F$ would have to be supplied, but even an ordering fixed by some convention would not prevent the evolution from sometimes taking hermitian elements to non-hermitian elements.

This latter problem: the ordering of factors and the hermiticity is neatly solved by Feynman’s approach of quasi-probabilities. He expands all qubit operators in a special basis of four hermitian operators $F(\xi) \in M_2$, $\xi \in \{++,+-,+-,-+\}$:

$$F_{uv} = \left(\begin{array}{cc} (1 + u)/2 & v(1 - iu)/4 \\ v(1 + iu)/4 & (1 - u)/2 \end{array}\right), \quad (u,v = \pm 1). \tag{39}$$

The expectations $f_\rho(\xi) = \text{tr}(\rho F(\xi))$ of these operators are the analogs of the Wigner function (see [21] for later elaborations on Wigner functions in finite dimension). Of course, by taking tensor products of these operators we get Wigner functions for multi-qubit systems. Now we can expand the transition rule for a single cell in Wigner operators:

$$T_0(F(\eta_0)) = \sum_{\xi_N} M(\eta_0|\xi_N) \bigotimes_{x \in N} F(\xi_x), \tag{40}$$

with the transition quasi-probabilities $M(\eta_0|\xi_N)$. These are usually not positive, but this is a minor inconvenience as long as the physical transition operator $T$ is positive. Equation (11) is just an expansion of the local rule in a basis of Wigner operators, so a local rule is completely equivalent to a set of transition quasi-probabilities. The difference between the quasi-probability approach and ours is how the global rule is constructed. Let us consider, for simplicity, the image of a two-site observable $F(\eta_1) \otimes F(\eta_2)$ under a one-dimensional nearest neighbor automaton. According to (35), transition probabilities must be combined as

$$T_{\text{qm}}(F(\eta_1) \otimes F(\eta_2)) = \sum_{\xi_0,\xi_1,\xi_2,\xi_3} M(\eta_1|\xi_0,\xi_1,\xi_2) M(\eta_2|\xi_1,\xi_2,\xi_3) \times F(\xi_0) \otimes F(\xi_1) \otimes F(\xi_2) \otimes F(\xi_3). \tag{41}$$

We can extend this to arbitrarily large configurations to get the time evolution of an automaton in the Heisenberg picture. Since the transition quasi-probabilities are real, this evolution will automatically preserve hermiticity, and since $\sum_\xi F(\xi) = 1$ all normalization and locality properties will automatically come out correctly. Of course, there will be no operator ordering problem, since we multiply at the level of functions, and all this will
work for probabilistic irreversible and reversible transition rules alike.

On the other hand, under the homomorphism $T$ the tensor product $F(\eta_1) \otimes F(\eta_2)$ is evolved to

$$T(F(\eta_1) \otimes F(\eta_2)) = \sum_{\xi_0, \xi_1, \xi_2} M(\eta_1 | \xi_0, \xi_1, \xi_2) M(\eta_2 | \xi_1, \xi_2, \xi_3)$$

$$\times F(\xi_0) \otimes F(\xi_1) F(\xi_2) \otimes F(\xi_3)$$

(42)

Then $U = U^\dagger$, iff $F(\xi) F(\eta) = \delta_{\xi \eta} F(\xi)$, which is obviously true for the minimal projections in a classical observable algebra, but obviously false for the Wigner operators. So the automata studied in this paper are not (or not in general) representable as quasi-probabilistic CAs.

Feynman uses the approach based on (41) only as a caricature of a quantum process. He points out that negative transition quasi-probabilities exclude a simulation of the global time step by successive independent random trials. For him this indicates the increased complexity of quantum computation.

Whether or not this approach works as a definition of (possibly also irreversible) QCAs hinges on the question of positivity. Non-positive transition probabilities would not be serious if they lead to the construction of a legitimate (i.e., completely positive) global transition rule. Unfortunately, however, there is no indication that quantum positivity improves in the passage from local to global rule. This can be seen already for a simple phase gate array, i.e., (P) in Fig. 10. For generic phase angle $\varphi$ neither the local transition nor the global transition e.g., the expression (42), have positive transition quasi-probabilities, although, of course, they correspond to completely positive operations. On the other hand, the two-site transition rule (41) takes some positive operators into non-positive ones.

An interesting special case occurs for phase angle $\phi = \pi$. In that case, the local rule does give rise to positive, and even deterministic transition quasi-probabilities. They belong to a classical deterministic CA, which like the phase gate QCA is its own inverse. But if it is applied as in (41), it violates positivity.

B. Watrous et al.

One of the first serious attempts at the definition of QCAs was by Watrous [6]. It is based on another “quantization” of the transition probability formula (43), inspired by Feynman’s notion that in quantum theory one must replace probabilities by amplitudes. Thus one tries a product formula like (43) for the transition amplitudes, presumably defining in this way the unitary transition operator for the whole process:

$$U(\alpha|\beta) = \prod_x u(\alpha_x|\beta_{N+x})$$

(43)

where $a, b$ are classical configurations, labelling the basis states of the QCA, and $b_{N+x}$ is the configuration $b$ restricted to the neighborhood of $x$. The function $u$ plays the role of the local transition rule. Basically the same definition is also used in van Dam [7], where it is phrased as an assignment of a a product vector to every basis state in the computational basis. Further work in this approach is to be found in [8] and in the textbook [8], or a recent introduction [27]. For the sake of discussion let us call an automaton defined by (43) a WQCA. There are several problems with this formula:

1. The infinite product may not be defined. This may be resolved by either introducing a “quiescent state” which is invariant under the evolution, and considering only superpositions of configurations which are quiescent outside a finite region $\mathcal{R}$, or to look at periodic boundary conditions only $\mathcal{R}$. Either approach works, but none of these workarounds is necessary in our definition.

2. $U$ from (43) has no reason to be unitary, and most of the time it isn’t. In other words, there is no straightforward way of characterizing those local transition amplitudes $u$ for which the formula does indeed define an isometric (or stronger: a unitary) operator, in which case the rule is called “well-formed” (or unitary). Whereas positivity and normalization of the local rule $M$ on the right hand side of (43) guarantee the corresponding properties for the global evolution, no equally simple criterion exists for well-formedness (but see [7] for algorithms in the one-dimensional case).

3. Many unitary operators are not of the form (43).

To begin with, the definition depends on the choice of a preferred basis. In general, the product of two WQCA unitaries need not be a WQCA (with larger neighborhood), and the inverse of a WQCA may fail to be a WQCA. This makes it hard to build a general theory on this definition.

To get an example of these phenomena note that a necessary condition for a unitary of Watrous form is that the computational basis states are mapped to product states. Moreover, if we follow the unitary operator by a site-wise unitary rotation, or precede it by a product of phase gates (i.e., introducing additional phase factors independent of the output labels $a_x$), we stay in this class. But now consider a sitewise Hadamard rotation, followed by a product of phase gates. It is easy to verify that such a map does not take the computational basis states to product states (or Briegel’s one-way computers would not work.) So this is not a WQCA, although it is the product of two WQCAs, and its inverse is also a WQCA.

4. Even in the cases where the formula does work, such as, e.g., for the multiplication by local phases,
the size of the neighborhood in [13] is not the neighborhood scheme describing the propagation of observable effects (the $\mathcal{N}$ of our definition), but rather the $\mathcal{N}$ from Section 11.1A. In fact, it is not even clear whether a WQCA is necessarily local in our sense. We did not manage to exclude the possibility that a local measurement after one time step might allow inferences about arbitrarily distant modifications of the state.

5. in the original paper [6], Watrous also looks at partitioned automata. Since we prove that all QCAs can be obtained by a partitioning scheme, it might seem that WQCA$\supset$QCA, in seeming contradiction to the Example in 3 above. However, Watrous uses only a special case of partitioning, namely a unitary followed by a permutation of subcells. Only if we extend the class of WQCAs and include all their products, we get all QCAs.

To summarize: Judged by the criteria in the introduction, the notion of Watrous is not a satisfactory formalization of the idea of quantum cellular automata. What is lacking is the easy passage from local to global rules, and from global axiomatic to local constructive description. For all problems involving the iteration of automata, the fact that the class is not closed under composition and inverse, puts a premature end to studies based on WQCAs.

C. Richter and Werner

As mentioned earlier, the observable-based approach underlying our definition was first used in [14] by one of us, but with a focus on the irreversible case. In that paper partitioning (dissipative cell evolution combined with permutation of subcells) was used to allow a free construction satisfying a global locality condition.

It is not so clear what should replace the axiomatic definition in the irreversible case. A possible condition is to just replace the local rule $T_0$ by a completely positive map, and insist on commutativity as before. This does define a global evolution step [14, 28]. In view of the reversible case this would seem like a good definition. However, it is again not clear whether the composition of two such transformations will again be of the same kind. Nor is it clear how to describe the class of transformations obtained by several such “simultaneous independent update” steps.

It turns out that the analysis of Theorem 8 can partly be repeated in the irreversible case, thereby reducing the possibilities somewhat. This line will be pursued elsewhere.

D. Wolfram

In a recent thick book [29], S. Wolfram has argued that the that the universe might be a big cellular automaton following simple rules (see also [31]). Wolfram uses only classical structures, expressing the belief, however, that quantum structures might emerge from classical rules generating sufficient complexity. Since Einstein failed with a program like that (he thought of overdetermined non-linear field equations, rather than CAs) it would be nice to see the details worked out.

E. Quantum random walks

The term “Quantum cellular automaton” has sometimes been used [31, 32, 33, 34] for a unitary evolution of a particle on a discretized space. The total Hilbert space of such a system is $\ell^2(\mathbb{Z})$, the space of square summable complex functions on the lattice, i.e., the direct sum rather than the tensor product of the one-cell spaces. The classical analogue of such a system is a single classical particle moving on a lattice, e.g., in a random walk. Therefore much better terminology to call these quantum systems quantum random walks, rather than cellular automata. Such systems have been proposed for purposes of quantum computation, in particular for search problems on graphs (see [35] for a review).

Quantum random walks require localization properties not unlike those of QCAs. To see the connection it is interesting to consider the connection between classical random walks and CAs: A random walk can be seen as a special CA, with each cell either empty or occupied, started in a configuration with exactly one occupied cell. Of course, the overall CA dynamics should respect this constraint. Because the CA rule is local we can then also put arbitrarily many particles on the lattice, and the dynamics is well-defined by the random walk, as long as the particles do not collide. What happens on collision is a piece of information which must be supplied in order to make a random walk into a CA, i.e., in order to pass from a random walk to a (possibly “interacting”) diffusion.

Consider a QCA with a special “empty” state specified for the single cell algebra. This means that we can define a global quantity particle number, which ought to be conserved by the QCA. Technically this is the infinite sum of 0’s and 1’s, and not a well defined observable. However, we can consider this formal sum as a lattice interaction generating the time evolution of “gauge transformations”, acting as an infinite product of unitaries, as in Section 11.1A. For a QCA commuting with such transformations, the “one-particle” Hilbert space can be defined, and the QCA dynamics restricted to this subspace is a unitary evolution of the random walk type. Note that we have not assumed that the dimension $d$ of the one-site algebra is 2, i.e., occupied cells (“particles”) may have an internal structure. This turns out to be necessary: a standard classical random walk, with only
the empty/occupied distinction and nearest neighbor interaction cannot be reversible. Similarly, a unitary on $L^2(\mathbb{Z}^2)$ cannot be strictly local \cite{31}, and we do need internal states $\mathbb{B}$. If there is only one particle, this is the same as saying that we have only the empty/occupied distinction for the cells, but we have also a “quantum coin” which helps determining the steps.

The standard model of a quantum random walk \cite{32} uses a qubit coin, i.e., three states for the QCA. All random walks with such a coin are parameterized by a single unitary $2 \times 2$-matrix $U$: we can describe the internal states (“chirality” \cite{34}) as “go right” and “go left”. A trivial, but globally well-defined evolution step is defined by following these instructions. The general case arises by following this with a sitewise unitary rotation by $U$, representing the quantum coin flip.

Now the question arises: can we consider such random walks as the one-particle component of a QCA allowing arbitrarily many particles? Indeed this is possible, even in many ways, and it would be very interesting to classify all possibilities, hence all “interactions”. One possibility is to second quantize the random walk, which leads to a Boson system allowing, at each site, an arbitrary number of particles. It is clear from the formalism of second quantization that all the locality properties required of a QCA are then satisfied. Clearly, this is the non-interacting option. If we insist on finitely many states per cell we introduce some kind of hard core interaction. A trivial way of doing it with four states is this: Consider two infinite qubit chains, called the left moving and the right moving chain. The “free” time evolution $S$ is indeed shifting the two chains separately according to this description. Now at each lattice site we take the right moving and the left moving one-site algebras together to define a single cell of the QCA, with the four states labelled ‘empty’, ‘R’, ‘L’, and ‘RL’. We then select a unitary $U$ leaving the empty and the doubly occupied state invariant, but shuffling the ‘R’ and ‘L’ states as before. Clearly, the combination of the free evolution $S$ with the sitewise application of $U$ defines a QCA whose one-particle sector is the given random walk.

F. Spacetime localized algebras

A quantum field theory can be considered from two equivalent points of view. On the one hand one can consider the fields at some time fixed time as the basic dynamical variables, e.g., the Cauchy data at time zero. On the other hand, for the discussion of relativistic causality, it is convenient to consider as fundamental the family of algebras $\mathfrak{A}(O)$ associated with the measurements in some space-time region $O$ \cite{12}. Similarly, one can look at a QCA from these two points of view, the “Cauchy data” point of view being what we described so far. For the space-time view consider the extended lattice $\mathbb{Z}^{s+1}$ of space-time points $(x, t)$, with $x \in \mathbb{Z}^s$, the same spatial lattice as before, and $t \in \mathbb{Z}$ a discrete time point.

The global C*-algebra will be the same as before, but we introduce additional subalgebras, namely

$$A_{x,t} = \mathcal{T}^{-t}(A_x).$$

(44)

Since $T$ commutes with lattice translations we can define a joint set of space-time translations $T_{x,t}$, combining a lattice translation by $x$ with $T^{-t}$. For any subset $O \subset \mathbb{Z}^{s+1}$ we define $\mathfrak{A}(O)$ as the C*-algebra generated by all the $A_{x,t}$ with $(x, t) \in O$. In order to study the localization properties of these algebras, let us say that a sequence of lattice points

$$(x_0, t_0), (x_1, t_0 + 1), (x_2, t_0 + 2), \ldots, (x_N, t_N)$$

(45)

is (forward) timelike, if $x_{k+1} - x_k \in \mathbb{N}$ for all $k$. Then we define two regions $O_1, O_2 \subset \mathbb{Z}^{s+1}$ to be spacelike separated (notation: $O_1 \not\subset O_2$), if no timelike curve passes through some point of $O_1$ and also through some point of $O_2$. Moreover, we say that $O_1$ is causally dependent on $O_2$ (notation: $O_1 \prec O_2$), if every timelike curve which passes through (any point of) $O_1$ also passes through $O_2$.

Then it is clear that $O_1 \prec O_2$ implies that $\mathfrak{A}(O_1)$ and $\mathfrak{A}(O_2)$ commute elementwise. Moreover, if $O_2$ is a finite set of lattice points $(x, t)$, all with the same $t$, and if $O_1 \prec O_2$, then $\mathfrak{A}(O_1) \subset \mathfrak{A}(O_2)$.

Conversely, if we have a net of local algebras $\mathfrak{A}(O)$, defined for arbitrary finite subsets $O$ of the spacetime-lattice, if the spacetime translations act by automorphism of the total algebra such that $T_{(x,t)}(\mathfrak{A}(O)) = \mathfrak{A}(O+(x,t))$, and that the above locality properties hold, then the time zero algebras form a QCA in the sense of Section 11.

This way of viewing QCAs may indeed be useful for making the connection to relativistic field theories, or for a detailed study of the growth of localization regions.

G. Non-commuting cells

As is standard in quantum theory we described the cells of the automaton as subsystems in the usual tensor product sense. In a slightly more axiomatic style we could have postulated, that arbitrary measurements in separate cells can be carried out jointly, implying the commutation between the different cells. While this is certainly very natural, more general commutation rules between cells may be considered. An obvious example are anti-commutation rules, i.e., we could think of a Fermi gas on a lattice. This would, of course, change the requirements on local rules, but it is quite clear how to adapt our definition to that case.

Another very interesting deviation from commuting cells is studied in \cite{37}, in connection with non-commutative analogs of 2-surfaces with constant negative curvature, the sine-Gordon equation, and 2-dimensional lattice systems in magnetic field (Hofstadter butterfly). Roughly speaking the structure investigated has has a single variable, say a unitary $Q_x$, at each cell “xz”. Non-commutativity comes in, because any pair of neighboring
unitaries forms a discrete Weyl system. At distances $\geq 2$ the variables commute. It is clear that (reversible) dynamical rules can be described exactly along the lines of our definition, as automorphisms respecting this algebraic structure, and also the localization (up to a finite enlargement of localization regions). Of course, this is not the place to explore such structures, and we point again to the book [37] for more material.

APPENDIX A: FINITE DIMENSIONAL C*-ALGEBRAS

Almost all the hard work in any textbook on C*-algebras goes into aspects of the theory, which become entirely trivial for finite dimensional C*-algebras. Of course, some algebras in this paper are infinite dimensional, notably the quasi-local C*-algebra describing the infinite system. But the key arguments use only the finite dimensional structure. Therefore we will give in this Appendix a quick summary of C*-algebra theory as it applies to the finite dimensional case.

In order to make the paper more accessible to communities in which algebraic terminology is less current (e.g., most theoretical physicists, and classical computer scientists) we start out with an extended glossary, in which the basic notions are defined and some basic facts are noted. This will be followed by some structure theorems which we need in the body of the paper. Of course, all this cannot replace a serious textbook. We recommend [11] [28] [68].

1. C*-Glossary

The operations making up the abstract structure of C*-algebras are inspired by those known from algebras of operators on a Hilbert space. In fact, every algebra of operators on a finite dimensional Hilbert space, which is also closed under taking adjoints, satisfies the definition, and every abstract C*-algebra is isomorphic to an operator algebra. The following list of relevant operations and concepts may serve as a glossary. The algebra under consideration is usually denoted by $\mathcal{A}$.

- **Addition** and multiplication by complex scalars. This makes $\mathcal{A}$ a vector space over $\mathbb{C}$, which we assume to be finite dimensional from now on.

- **Multiplication**. We denote the product by $AB \in \mathcal{A}$, when $A, B \in \mathcal{A}$. The product is distributive and associative (but not necessarily commutative). If the algebra is commutative or “abelian” the system under consideration is classical.

- The adjoint or “star operation” denoted by $A^* \in \mathcal{A}$, when $A \in \mathcal{A}$. This is conjugate linear (or “antilinear”), which means that $(\lambda A)^* = \bar{\lambda} A^*$, and $(A+B)^* = A^* + B^*$. The adjoint satisfies $(AB)^* = B^* A^*$. Physicists often write $A^\dagger$ for the adjoint.

- The **norm**, which is a positive number $\|A\|$ associated with each $A \in \mathcal{A}$. With respect to the algebraic structures, the norm satisfies $\|A + B\| \leq \|A\| + \|B\|$, $\|\lambda A\| = |\lambda| \|A\|$, $\|AB\| \leq \|A\| \|B\|$ and $\|A^* A\| = \|A\|^2$. $\|A\| = 0$ implies $A = 0$. In contrast to the general case, the norm is uniquely determined by the algebraic structures.

- **An identity**. In contrast to the general case, in finite dimensional C*-algebras there is always a unique element $1$ satisfying $1A = A1 = A$.

- A **homomorphism** between C*-algebras is a map $\Phi : \mathcal{A} \to \mathcal{B}$ between C*-algebras, preserving the algebraic structures. That is, $\Phi$ is linear, $\Phi(AB) = \Phi(A)\Phi(B)$, and $\Phi(A^*) = \Phi(A)^*$. The latter property is sometimes emphasized by speaking of $*$-homomorphisms. Homomorphisms $\Phi : \mathcal{A} \to \mathcal{A}$ are called endomorphisms of $\mathcal{A}$, and if an inverse homomorphism exists, $\Phi$ is called an isomorphism or an automorphism (if $\mathcal{A} = \mathcal{B}$). For general homomorphisms, $\Phi(1)$ is a projection in $\mathcal{B}$. If $\Phi(1) = 1$, we call it unital.

- **An ordering**. We write $A \geq 0$, if there is a $B \in \mathcal{A}$ such that $A = B^* B$. The set of positive elements is a convex cone in the set of hermitian ($A^* = A$) elements. In an operator algebra, the positive elements are precisely those hermitian ones with all eigenvalues non-negative.

- The **center** of $\mathcal{A}$ is the subalgebra $Z(\mathcal{A}) \subset \mathcal{A}$ of elements $Z$ such that $ZA = AZ$ for all $A \in \mathcal{A}$.

- A **state** on $\mathcal{A}$ is a linear functional $\omega : \mathcal{A} \to \mathbb{C}$ which is positive (i.e., $A \geq 0$ implies $\omega(A) \geq 0$) and normalized (i.e., $\omega(1) = 1$).

- A **trace** on $\mathcal{A}$ is a positive linear functional $\tau$ such that $\tau(AB) = \tau(BA)$.

- A positive linear functional $\omega$ is called faithful if $A \geq 0$ and $\omega(A) = 0$ imply $A = 0$. Every finite dimensional C*-algebra has a faithful trace. On an operator algebra, the usual trace of operators (which we will denote by tr) is an example.

- Given a faithful trace $\tau$, every positive linear functional can be written as $\omega(A) = \tau(\rho A)$, for a unique $\rho \in \mathcal{A}$, $\rho \geq 0$, which is called the density operator of $\omega$ with respect to $\tau$. $\omega$ is also a trace iff $\rho \in Z(\mathcal{A})$.

- An element $P \in \mathcal{A}$ is called a projection if $P^* = P = P^2$. It is called a minimal projection if for any projection $Q$, $Q \leq P$ implies $Q = 0$ or $Q = P$.

- The **direct sum** $\mathcal{A} = \bigoplus_{\mu} \mathcal{A}_{\mu}$ of a finite collection of finite dimensional C*-algebras $\mathcal{A}_{\mu}$ is the vector...
space direct sum, i.e., elements are tuples of components $A_\mu \in A_\mu$, with componentwise algebraic operations. In operator algebras each term in the sum corresponds to a diagonal block in a block matrix decomposition.

- The tensor product $A = \bigotimes_\mu A_\mu$ is the vector space tensor product, with product and adjoint defined as the unique linear (resp. conjugate linear) extensions of $(\otimes_\mu A_\mu)(\otimes_\mu B_\mu) = \otimes_\mu (A_\mu B_\mu)$ and $(\otimes_\mu A_\mu)^* = \otimes_\mu A_\mu^*$. In operator algebras one forms this product by taking first the tensor products of the underlying Hilbert spaces, and taking the algebra generated by all tensor product operators.

The first four items on this list are the definition of C*-algebras. Note that order and unit are explicitly defined in terms of the algebraic structure (linear operations, multiplication and adjoint), and the norm is also defined explicitly as

$$\|A\| = \inf\{\lambda > 0 | \exists_B A^*A + B^*B = \lambda^2 I\} \quad (A1)$$

It might thus seem superfluous to list the norm among the defining elements. In the infinite dimensional case it is needed, of course, to formulate the topological completeness requirement (and completeness is needed in turn to construct $B$ in (A1)). However, even in the finite dimensional case the implication $(\|A\| = 0) \Rightarrow (A = 0)$ carries non-trivial information by excluding the existence of nonzero elements $A_i$ such that $\sum_i A_i^* A_i = 0$.

2. C*-structure

Consider a single Hermitian element $A \in A$. Then since $A$ is finite dimensional, the powers $A^n$ must be linearly dependent, i.e., there is a characteristic polynomial $p(A) = \sum_k c_k A^k = 0$. From this one readily constructs polynomials $p_\ell$ such that $p_\ell(A)$ is a projection, and

$$A = \sum_\ell a_\ell p_\ell(A) \quad (A2)$$

where $a_\ell$ are the distinct roots of $p(a) = 0$. This is called the spectral theorem. It implies, in particular, that any finite dimensional C*-algebra has many projections (which may fail in infinite dimension).

This fact will be used in the following fundamental structure theorem. Recall that by $M_n$ we denote the algebra of complex $n \times n$ matrices.

**Proposition 11** Every finite dimensional C*-algebra $A$ is characterized uniquely up to isomorphism by a finite sequence $n_1 \geq n_2 \geq \cdots \geq 1$ of numbers such that

$$A \cong \bigoplus_\mu M_{n_\mu}. \quad (A3)$$

The basic idea of the proof is to consider the center of $A$, which is a finite dimensional abelian C*-algebra. The minimal projections $z_\mu$ of the center decompose the algebra into a direct sum $A = \bigoplus_\mu z_\mu A$, in which each of the summands has trivial center. The building blocks $z_\mu A$ are then seen to be isomorphic to full matrix algebras $M_{n_\mu}$, where $n_\mu$ is the maximal number of mutually orthogonal projections in $z_\mu A$.

**Proposition 12** If $\Phi : M_d \to \bigoplus_\mu M_{n(\mu)}$ is a *-homomorphism such that $\Phi(1) = 1$, each $n(\mu)$ has to be divisible by $d$.

By considering the composition of the given homomorphism with the projection onto one summand, which is also a homomorphism, we can consider the case of a single summand. Thus $\Phi$ becomes a representation of $M_d$ on a Hilbert space of dimension $d(\mu)$, which can be decomposed into irreducible representations. It is a basic property of $M_d$, however, that all its irreducible representations are unitarily equivalent to the defining representation on $C^d$, so $n(\mu)$ must be $d$ times the multiplicity (number of isomorphic irreducible summands) of this representation.

**Proposition 13** If $A \cong \bigoplus_\mu M_{n(\mu)}$ and $B \cong \bigoplus_\nu M_{n(\nu)}$ are commuting subalgebras of $B(H)$, the algebra $AB$ is also decomposed into direct summands, each of which arises by multiplying a summand form each of the algebras. These occur with integer multiplicities $r_{\mu\nu} \geq 0$ such that

$$\sum_{\mu\nu} r_{\mu\nu} n(\mu)n(\nu) = \dim H. \quad (A4)$$

Let $A_\mu \in M_{n(\mu)} \subset A$ and $B_\nu \in M_{n(\nu)} \subset B$ be elements from the respective blocks. Then $A_\mu \otimes B_\nu \to A_\mu B_\nu$ is a representation of $M_{n(\mu)} \otimes M_{n(\nu)} \cong M_{n(\mu)n(\nu)}$ on $H$, which may however be zero since we cannot guarantee that it preserves the identity. The rest of the argument is as for the previous proposition.

**APPENDIX B: ACKNOWLEDGEMENTS**

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[1] R. Feynman, Simulating physics with computers, Int. J. Theor. Phys. 21 (1982) 467-488. Reprinted in A.J.G. Hey (ed.), Feynman and Computation, Perseus Books 1999.

[2] O. Mandel, M. Greiner, A. Widera, T. Rom, T.W. Hänsch, and I. Bloch, Coherent transport of neutral atoms in spin-dependent optical lattice potentials, Phys. Rev. Lett. 91, 010407 (2003)

[3] R. Dumke, M. Volk, T. Muether, F.B.J. Buchkremer, G. Birk, and W. Ertmer, Microoptical Realization of Arrays of Selectively Addressable Dipole Traps: A Scalable Configuration for Quantum Computation with Atomic Qubits, Phys. Rev. Lett. 89, 097903 (2002) and quant-ph/0110140

[4] Further away are proposals based on arrays of quantum dots, which are also published under the heading "quantum cellular automata". These are ideas for new hardware for classical computing, possibly replacing CMOS technology. In order to avoid confusion with the ideas in which quantum coherence plays a key role (as it does in our paper), many authors from that community are now using the more precise term "quantum dot cellular automata". For an overview see the home page of the Notre Dame group (www.nd.edu/~qcahome), or: P.D. Tougaw, C.S. Lent, Logical devices implemented using quantum cellular automata, J.Appl.Phys. 75 (1994) 1818.

[5] S. C. Benjamin, Schemes for parallel quantum computation without local control of qubits, Phys. Rev. A 61 020301 (2000)

[6] J. Watrous: On one-dimensional quantum cellular automata. In Proceedings of the 36th Annual Symposium on Foundations of Computer Science, 1995, pp. 528–537.

[7] W. van Dam: Quantum cellular automata, Master Thesis, Computer Science Nijmegen, Summer 1996

[8] J. Gruska: Quantum Computing, (McGraw-Hill, Cambridge 1999). QCAs are treated in Section 4.3.

[9] C. Dür and M. Santha: A decision procedure for unitary linear quantum cellular automata, quant-ph/9904007. C. Dür, H. LeTanH and M. Santha, A decision procedure for well-formed linear quantum cellular automata, Rand. Struct. Algorithms 11, 381-394 (1997) and cs.DS/9906024

[10] G. K. Brennen and J. E. Williams, Entanglement dynamics in 1D quantum cellular automata, quant-ph/0306056

[11] O. Bratteli and D. Robinson: Operator algebras and quantum statistical mechanics, vol. I (Springer 1979)

[12] A C*-algebraic framework was also applied to QCAs in a recent thesis. However, it was applied to the state side, rather than the observables, making locality properties harder to see. K. Paschen: Über Reversibilität, Nicht-Determiniertheit und Quantenrechnen in Zellulärautomaten, Dissertation in Informatik (PhD Thesis in Computer Science), Karlsruhe 2002

[13] R. Haag: Local quantum physics, Springer 1996

[14] S. Richter and R.F. Werner, Ergodicity of quantum cellular automata, J. Stat. Phys. 82 (1996) 963-998 and cond-mat/9504001

[15] J. Kari, On the circuit depth of structurally reversible cellular automata, Fund. Inform. 34 (2003) 1-15

[16] The basic concepts in this paragraph work in any lattice structure. In fact, they do not even require translation invariance and could be formulated for possibly different spins (given by possibly infinite dimensional C*-algebras) localized on the nodes of a finite or infinite graph.

[17] R. Raussendorf, D. E. Browne and H.-J. Briegel, The one-way quantum computer - a non-network model of quantum computation, J. Mod. Opt 49, 1299 (2002).

[18] D. Richardson, Tessellation with local transformations, J.Comput.Syst.Sci. 6 (1972) 373-388

[19] What appears here as a pathology is allowed in the (periodic boundary version) of Watrous QCAs, i.e., the Wrapping Lemma fails for that structure. A more systematic study of the possibility shown by our example was carried out in S. Inokuchi, Y. Mizoguchi, Generalized partitioned quantum cellular automata and quantization of classical CA, quant-ph/0312102

[20] S. Lloyd, A potentially realizable quantum computer, Science 261, 1569-1571 (1993)

[21] We follow this terminology, although it is not clear what Clifford had to with this. In field theory these transformations would be called "quasi-free", or "Bogolyubov automorphisms", in phase space quantum mechanics "metaplectic transformations".

[22] D. Schlingemann, R.F. Werner, The structure of Clifford quantum cellular automata, in preparation.

[23] T. Toffoli and M. Margolus, Invertible Cellular automata: a review, Physica D45(1990) 229-253

[24] The support algebra of a single element, an interaction Hamiltonian was also introduced under the name "interaction algebra" by P.Zanardi: Stabilization of quantum information: a unified dynamical-algebraic approach, quant-ph/0203008

[25] K.S. Gibbons, M.J. Hoffman, W.K. Wootters, Discrete phase space based on finite fields, quant-ph/0401155

[26] J. P. Paz: Discrete Wigner functions and the phase space representation of quantum teleportation, quant-ph/0204150

[27] B. Aoun, M. Tarifi, Quantum cellular automata, quant-ph/0401123

[28] M. Takesaki, Theory of operator algebras, I, Springer 1979

[29] S. Wolfram, A new kind of science, (Self-published, Wolfram Media Inc. 2002)

[30] K. Zuse, Rechnerer Raum, Schriften zur Datenverarbeitung, Band 1, Vieweg, Braunschweig 1969.

[31] G. Grössing and A. Zeilinger, Quantum cellular automata, Complex Systems 2, 197–208 (1988)

[32] I. Bialynicki-Birula, Weyl, Dirac, and Maxwell equations on a lattice as unitary cellular automata, Phys. Rev. D 49, 6920–6927 (1994)

[33] D. A. Meyer, From quantum cellular automata to quantum lattice gases, J. Stat. Phys. 85, 551–574 (1996)

[34] N. Konno, K. Matsuda, T. Soshi, H.J. Yoo, Quantum walks and reversible cellular automata, quant-ph/0403107

[35] J. Kempe, Quantum random walks: an introductory overview, Contemp.Phys. 44 (2003) 307 - 327

[36] D. A. Meyer: Unitarity in one dimensional nonlinear quantum cellular automata, quant-ph/9603023. From quantum cellular automata to quantum lattice gases, J.Stat.Phys. 85 (1996) 551–574

[37] A.I. Bobenko, R. Seiler (eds.), Discrete integrable ge-
ometry and physics, Clarendon Press, Oxford 1999. The book has several articles connecting to the structure mentioned in the text. It is best to pick up the pointers in the introduction by the editors.

[38] J. Dixmier, *C*-algebras, North Holland 1977