Quantum Cellular Automata

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Abstract: Quantum Cellular Automata (QCA) are lattices with a quantum system at each site that have discrete time evolution with finite information propagation speed. They have been showed very promising, for instance, as a model for lattices evolving via time-dependent Hamiltonians. In this work we will explain that 1D QCA are equivalent to Matrix Product Unitaries and classify them according to their information flow. This allows to realize that all 1D QCA are compositions of finite depth quantum circuits and shift operations.

I. INTRODUCTION

Classical cellular automata are systems of discrete variables at each site of a lattice, which evolve in time via iterations of a local rule applied over all sites. Interestingly, even when the local rule is simple it is possible to observe very complex dynamics. For example, it has been proved that they can efficiently simulate Turing machines, traffic models, biological pattern formation or fluids dynamics [1]. This work is focused on quantum versions of classical cellular automata, that is, lattices systems of identical particles evolving in discrete time by locality preserving unitary transformations [2].

It has been shown that quantum cellular automata (QCA) are able to efficiently simulate quantum circuits [3, 4]. They could therefore be an alternative quantum computation model. An advantage they would have over the circuit model is that the computation could be carried out with homogeneous operations applied over all particles, and individual particles operations would not be necessary. QCA have the potential to simulate quantum field theory dynamics [5], lattices evolving via time-dependent Hamiltonians [6] or quantum lattice gases [7]. But QCA are interesting in their own right as we will see here. In principle, a QCA could be defined on any graph. We will however limit ourselves to one-dimensional QCA with qudits at the lattice sites.

This work is organized as follows. In Section II QCA will be defined mathematically and some examples will be given. In Section III matrix product unitaries (MPU) will be introduced and shown to provide a useful representation of QCA. Section IV is devoted to the classification of QCA through an index theory that characterises their information flow. We provide an outlook in Section V.

II. QUANTUM CELLULAR AUTOMATA

We consider a lattice \mathcal{L} , which could be infinite or finite. When the lattice is finite, we will assume periodic boundary conditions. We identify each site x with a Hilbert space \mathcal{H}_x . It would only be natural to study QCA using the tensor product Hilbert space $\mathcal{H} = \bigotimes_{x \in \mathcal{L}} \mathcal{H}_x$. However, such tensor product spaces bring mathematical difficulties when the lattice is infinite. To avoid them, a common strategy is to work in Heisenberg picture instead of Schrödinger picture, and exploit locality. For this reason, our description of a QCA will sometimes be in terms of C^* -algebras of local operators, $\{\mathcal{A}_x : x \in \mathcal{L}\}$, instead of local Hilbert spaces of states, $\{\mathcal{H}_x : x \in \mathcal{L}\}$. The algebra of operators associated with a region $\Lambda \subset \mathcal{L}$ is defined in terms of those of each lattice site as $\mathcal{A}_{\Lambda} = \bigotimes_{x \in \Lambda} \mathcal{A}_x$. Such algebras act nontrivially on systems in Λ and as the identity on the rest of the lattice [8]. Then,

$$\mathcal{A}_{\mathcal{L}} = \bigcup_{\Lambda \subset \mathcal{L}} \mathcal{A}_{\Lambda}$$

is the algebra of local observables on the whole lattice, i.e. observables supported on finite regions of \mathcal{L} . The discrete dynamics of a QCA can be described by a local automorphism:

$$\alpha_x: \mathcal{A}_x \to \mathcal{A}_{\mathcal{N}(x)},$$

where $\mathcal{N}(x) \subset \mathcal{L}$ denotes a finite neighbourhood of x. This implies that the evolution is locality-preserving, that is, evolving an operator localized at x produces an operator whose support is contained in the neighbourhood $\mathcal{N}(x)$ of x, as illustrated in figure 1. For finite lattices there will be an unitary U such that $\alpha_{\mathcal{L}}(\cdot) = U^{\dagger}(\cdot)U$. However, not every automorphism can be constructed in this way for infinite lattices.

Besides, we will restrict ourselves to translationally invariant QCA, that is, $\alpha_x = \alpha$ for all x in \mathcal{L} . This allows us to assume, without loss of generality, that any QCA is a **nearest neighbour QCA**, i.e. $\mathcal{N}(x) \subseteq \{x - 1, x, x + 1\}$, which we can always achieve by blocking sites into large enough units; a supersite of k qudits will have an effective local dimension $d_{\text{eff}} = d^k$.



FIG. 1: QCA of radius equal to 2. Representation of an operator O localized at a site of a 1D lattice to which α is applied. $\alpha(O)$ is localized in a nearby region of 5 sites.



In this circuit, each box represents a two-qudit unitary gate. We are going to call **finite depth quantum circuits** (FDQC) those QCA built with a finite number of circuits layers (this means that when raising the number of qudits the number of layers does not increase). An example of a QCA that is not an FDQC is the right **shift**, represented as:



In Heisenberg picture the right shift QCA σ acts on an operator O located at site x as $\sigma(O_x) = O_{x+1}$. Obviously, the left shift is $\sigma^{-1}(O_x) = O_{x-1}$.

Margolus Partitioning. There is a mathematical way of writing any one-dimensional translationally invariant QCA, showed in [9]: the generalized Margolus partioning. It involves an ancillary lattice \mathcal{L}^a , that is, a complementary lattice that will help us in the application of the QCA but it must start and finish in a trivial state. A map from \mathcal{L} to \mathcal{L}^a and another map from \mathcal{L}^a to \mathcal{L} will be enough to describe any nearest neighbour QCA.

The key idea in this method is that \mathcal{L}^a slightly breaks translational invariance: dimensions of qudits at even sites (d_1) may be different than dimensions of qudits at odd sites (d_2) of the lattice \mathcal{L}^a . However, it must always be true that $d_1d_2 = d^2$, where d is the dimension of the qudits of the lattice \mathcal{L} .

Let $\{\mathcal{B}_x : x \in \mathcal{L}^a\}$ denote C^* -algebras supported on each site of \mathcal{L}^a . We define two (translationally invariant) maps:

$$\mu: \quad \mathcal{A}_{2x} \otimes \mathcal{A}_{2x+1} \to \mathcal{B}_{2x} \otimes \mathcal{B}_{2x+1}, \\ \nu: \quad \mathcal{B}_{2x-1} \otimes \mathcal{B}_{2x} \to \mathcal{A}_{2x-1} \otimes \mathcal{A}_{2x}.$$

This maps, μ and ν , are required to be unitary mappings between algebras of the same dimension, thus we can find suitable bases in each site such that $\mu(\cdot) = U_{\mu}^{\dagger}(\cdot)U_{\mu}$ and $\nu(\cdot) = U_{\nu}^{\dagger}(\cdot)U_{\nu}$, where U_{μ} and U_{ν} are unitary matrices (even when \mathcal{L} is infinite). Any QCA automorphism can be constructed applying a μ followed by ν at each site, $\alpha(\cdot) = \nu(\mu(\cdot)) = U_{\nu}^{\dagger}U_{\mu}^{\dagger}(\cdot)U_{\mu}U_{\nu}$. Figure 2 illustrates a construction of a QCA through this method.

For example, for a right shift, we have that $d_2 = d^2$ and $d_1 = 1$. Whereas for a FDQC, $d_2 = d$ and $d_1 = d$. Notice that for FDQC the ancillary lattice \mathcal{L}^a would not be needed and ν and μ would be automorphisms.

Following the notation of the circuits any onedimensional transitionally invariant QCA can represented as:



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FIG. 2: Representation of a nearest neighbour QCA constructed by the Margolus Partitioning method. Algebras \mathcal{A}_x supported on \mathcal{L} and algebras \mathcal{B}_x on \mathcal{L}^a .

The legs between the unitaries been drawn dashed to represent d_1 dimensions, dotted to represent d_2 dimensions and plain lines (input and output legs) correspond to the *d*-dimensional qudits at the physical lattice \mathcal{L} . This diagram would only represent an FDQC if dimensions of all legs where equal.

III. MATRIX PRODUCT UNITARIES

We now turn to matrix product unitaries (MPU). We consider again a one-dimensional finite lattice \mathcal{L} with a *d*-dimensional qudit at each site and periodic boundary conditions. A translationally invariant matrix product operator (MPO) is defined as:

$$\mathcal{O}^{(N)} = \sum_{\substack{i_1\dots i_N\\j_1\dots j_N}} c_{j_1\dots j_N}^{i_1\dots i_N} \left| i_1\dots i_N \right\rangle \left\langle j_1\dots j_N \right| \,, \tag{1}$$

the coefficients c are given by the expression:

$$c^{i_1\ldots i_N}_{j_1\ldots j_N} = \sum_{\alpha_1\ldots\alpha_N} \mathcal{T}^{i_1j_1}_{\alpha_1\alpha_2} \mathcal{T}^{i_2j_2}_{\alpha_2\alpha_3} \ldots \mathcal{T}^{i_Nj_N}_{\alpha_N\alpha_1} \,,$$

where \mathcal{T} is a rank-4 tensor with indices i, j (the physical ones) and α, β (the bond or auxiliary indices): $\mathcal{T}_{\alpha\beta}^{ij}$. As we have *d*-dimensional qudits *d* will be the rank of the physical indices (i, j = 1, 2, ..., d). The rank of the bond indices will be denoted *D*, and referred to as bond dimension $(\alpha, \beta = 1, 2, ..., D)$. Also, *N* is the number of sites of the lattice and $|i_1...i_N\rangle = \bigotimes_{x \in \mathcal{L}} |i_x\rangle$, where $|i_x\rangle$ is the state of the qudit at site *x*. Therefore, $\mathcal{O}^{(N)}$ can be seen as a matrix of $d^N \times d^N$ dimensions. MPO are commonly used to describe quantum spin systems and are suitable to simulate efficiently time evolution [10, 11].

An MPU is an MPO which is unitary for all lattice sizes [8], that is:

$$\mathcal{O}^{(N)\dagger}\mathcal{O}^{(N)} = \mathbb{1}^{\otimes N} \,. \tag{2}$$

This condition imposes very strong constraints on \mathcal{T} , we will call "tensor generating MPU" those tensors that meet these constrains. MPUs have been used to describe evolution of one-dimensional spin lattices nearest neighbour Hamiltonians [12]. It is very useful to use a graphic notation to work with operators (and states) constructed from contraction of tensors [11]. As a useful example, we will represent a vector v_i as a box with a leg, a matrix M_{ij} as a box with two legs and the tensor $\mathcal{T}_{\alpha\beta}^{ij}$ as a box with four legs:

$$-v$$
 $-M$ $-\tau$

Vertical legs of $\mathcal{T}_{\alpha\beta}^{ij}$ represent the physical indices and the horizontal ones the bond indices. Joining two legs will represent contraction, thus multiplication and the trace is depicted as follows:

$$M\vec{v} = M_{ij}v_j = -M - v = -Mv$$
$$AB = A_{ij}B_{jk} = -A - B - -AB - tr(M) = M_{ii} = -M$$

Then eq. 1 can be written as:

where the bent legs (at the beginning and the end) indicate that these two are also connected, i.e. periodic boundary condition. If we denote $\overline{\mathcal{T}}$ the resulting tensor after transposing the physical indices and conjugating all coefficients of \mathcal{T} , eq. 2 can be now represented as:

We will denote \mathcal{T}_k the blocking of $k \mathcal{T}$ tensors, that is:

where the rank of the thick legs indices is equal to d^k . The rank of horizontal legs is still equal to D.

Simple tensors.- We will say that \mathcal{T} is a simple tensor if there exist two tensors, a and b, that satisfy the following two conditions:

$$\begin{array}{c} \left[\overrightarrow{T} \\ \overrightarrow{0} \overrightarrow{0} \\ \overrightarrow{0} \overrightarrow{0}$$

Therefore, any simple tensor generates MPU, since:

i.e. condition of eq. 2 is satisfied.

Conversely, it can be proved that for any tensor \mathcal{T} generating MPU there is a $k_0 \leq D^4$ such that for any $k \geq k_0$, \mathcal{T}_k is simple. This means that by blocking a tensor generating MPU one can always get a simple tensor. In addition, once we have a simple tensor, if we keep blocking

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the resulting tensor will remain simple, [13, Theorems 3 and 5] and [14, Theorem 2].

Tensors \mathcal{T} can be reshaped and written as $dD \times dD$ matrices. In fact, depending on how the indices are combined, two different matrices can be obtained. We will call M_1 the matrix obtained by combining the left auxiliary and down physical indices as well as the right auxiliary and up physical indices, and M_2 the other combination of the physical and auxiliary indices. Let $M_i = V_i^{\dagger} D_i U_i$ (i = 1, 2) denote the singular value decomposition of these matrices, where V_i , U_i are isometries, and D_i is a positive diagonal matrix of dimension r for M_1 and dimension ℓ for M_2 . Thus r and ℓ are the rank of the matrices M_1 and M_2 . We will call r "the right rank" and ℓ "the left rank". It is immediate that we can find two matrices (or tensors) such that $M_i = \mathcal{X}_i \mathcal{Y}_i$ [14]. For M_1 we can represent this decomposition as:

$$-\underbrace{V_1}_{\mathbf{M}_1} = \underbrace{V_1^{\dagger}}_{\mathbf{M}_1} \underbrace{D_1}_{\mathbf{M}_1} \underbrace{U_1}_{\mathbf{M}_1} = \underbrace{V_1^{\dagger}}_{-\underbrace{\mathcal{M}_1}}$$

The diagonal double line means to combine the indices to build the matrix, the legs that are not separated by the diagonal are combined. The dotted legs mean that the rank of these legs is equal to r. And the rank of thick legs is equal to dD. At last step, the legs of \mathcal{X}_1 and \mathcal{Y}_1 have been uncombined into the originals. Thus, we can decompose \mathcal{T} as (for M_2 blue is used instead of red):

The dashed legs mean that the rank of these legs is ℓ . The ranks r and ℓ depend on each tensor \mathcal{T} generating MPU, however $rl = d^2$ if and only if \mathcal{T} is simple [14, Theorem 8]. Remember that d is the dimension of the qudits and, therefore, the rank of the physical indices, but after the blocking the dimension of the effective qudits increases.

To finish, we will define two operators u and v:

$$u = \underbrace{\underbrace{\mathcal{Y}_2}}_{1} - \underbrace{\underbrace{\mathcal{Y}_1}}_{1} = \underbrace{\underbrace{\mathcal{Y}_2}}_{1} - \underbrace{\underbrace{\mathcal{Y}_2}}_{1} = \underbrace{\underbrace{\mathcal{Y}_1}}_{1} - \underbrace{\underbrace{\mathcal{Y}_2}}_{1} = \underbrace{\underbrace{\mathcal{Y}_2}}_{1} - \underbrace{\underbrace{\mathcal{Y}_2}}_{1} - \underbrace{\underbrace{\mathcal{Y}_2}}_{1} = \underbrace{\underbrace{\mathcal{Y}_2}}_{1} - \underbrace{\underbrace{\mathcal{Y$$

These are unitary as shown in [14], again, if and only if \mathcal{T} is simple.

Equivalence with QCA. We can now show that any MPU is equivalent to a one-dimensional transitionally invariant QCA [14]. The automorphism associated with an MPU:

$$\alpha(\cdot) = \mathcal{U}^{(N)\dagger}(\cdot)\mathcal{U}^{(N)}$$

is a QCA, since $\mathcal{U}^{(N)}$ is unitary, and it can be seen that it commutes with the translation operator. Thanks to the conditions of eq. 3 it can be proved that the radius of this QCA would be less or equal than D^4 .

To prove the converse, we take the decomposition for \mathcal{T} and we immediately see that the following is true (if

 ${\mathcal T}$ is simple, which can always be achieved by blocking):



which is exactly the diagram we found at the end of section II for a nearest neighbour QCA. If we compare the legs of the two diagrams we see that: $r = d_2$ and $\ell = d_1$.

IV. INDEX THEORY

We are going to define an index that will assign a real number to each QCA. This index will classify the QCA, that is, two QCA have the same index if and only if there is a continuous path of QCA that joins them. The formalism of tensor networks, more specifically the equivalence of QCA with MPUs, will help us in this definition. We will clearly see that the index will measure the net amount of quantum information that flows. Intuitively one can realize that shifts add information flow while, a priori, FDQCs do not seem to introduce it. In other words, the QCA automorphisms form a group and the index will classify the different QCA into subgroups.

The index of a simple tensor \mathcal{T} is defined as [14]:

$$\operatorname{ind}(\mathcal{T}) = \frac{1}{2} \left[\log_2\left(r\right) - \log_2\left(\ell\right) \right] \,.$$

Since this index is defined for simple tensors, it might be necessary to do some blocking until \mathcal{T}_k becomes simple in order to compute $\operatorname{ind}(\mathcal{T})$.

As we have said, this index helps us classify QCA, therefore the index of \mathcal{T} should not change by blocking. That is, \mathcal{T}_{k_0} and \mathcal{T}_k should have the same index if $k \geq k_0$ and k_0 is the smallest k for which \mathcal{T}_k is simple. To prove this, we can write \mathcal{T}_k and do the decomposition as:

$$-\frac{1}{T_{k-k_0}} = -\frac{1}{T_{k-k_0}} + \frac{1}{T_{k_0}} = \frac{1}{t_{k-k_1}} + \frac{1}{t_{k_0}}$$

It is seen that the right rank $r_k \leq d^{k-k_0}r_{k_0}$. If we now write the \mathcal{T}_k as the result of blocking \mathcal{T}_{k_0} and \mathcal{T}_{k-k_0} (i.e., the reverse of what has been done previously), we see that for the left rank: $\ell_k \leq d^{k-k_0}\ell_{k_0}$. As \mathcal{T}_k is simple, $\ell_k r_k = d^{2k}$, inequalities become equalities, therefore:

$$\operatorname{ind}(\mathcal{T}_k) = \frac{1}{2} \log_2\left(\frac{r_k}{\ell_k}\right) = \frac{1}{2} \log_2\left(\frac{r_{k_0}}{\ell_{k_0}}\right) = \operatorname{ind}(\mathcal{T}_{k_0}).$$

Index Theorem.- Index, as defined above, is a complete topological invariant. That is, by changing continuously the coefficients of the tensor \mathcal{T} one cannot alter the index, and two tensors \mathcal{T} and \mathcal{T}' have the same index if and only if they are path-equivalent, i.e. there is a family of tensors $\mathcal{W}(x)$, where $x \in [0,1]$ such that $\mathcal{W}(0) = \mathcal{T}$ and $W(1) = \mathcal{T}'$ (ancillas may be added to one of the tensors). In proposition IV of [14] it is explained that this family exists and its ranks would be r(x) and $\ell(x)$ (continuous functions), but as ranks can only be integers they must be constant, and, therefore, the index should remain the same.

Another important property that can be seen is that the index is additive by tensoring and composition [14]:

$$\operatorname{ind}(-\Box + \otimes -\Box) = \operatorname{ind}(-\Box + \Box) = \operatorname{ind}(-\Box + \Box) + \operatorname{ind}(-\Box + \Box)$$
$$\operatorname{ind}(-\Box + \circ -\Box + \operatorname{ind}(-\Box + \Box)) = \operatorname{ind}(-\Box + \Box) + \operatorname{ind}(-\Box + \Box)$$

where the circle and the box represent two different tensors generating MPU.

Examples.- Let us look at two examples of index computation:

- **FDQC:** the ranks of 4 legs of the unitaries (*u* and *v*) representing a FDQC, γ , should be equal, therefore $r = \ell = d$ and $ind(\gamma) = 0$.

- Shifts: all the information flows in one direction, thus $\ell = 1$ and $r = d^2$ for the right shift ($\ell = d^2$ and r = 1for the left shift). This means that: $\operatorname{ind}(\sigma) = \log_2(d)$ for the right shift ($\operatorname{ind}(\sigma^{-1}) = -\log_2(d)$ for the left shift).

One of the most remarkable results that follows is that, as the index can only take certain values, there is no continuous path of tensors joining any FDQC with a shift (there is no path between a right shift and a left shift either) and shifts introduce information flow; any QCA can be expressed as a composition or tensoring of circuits and shifts (after blocking and adding ancillas) [15]. Therefore the index will show the logarithm of "net" shifts.

Alternative approach.- We close this section by presenting an alternative formula for the index [6], where the information theoretic interpretation is more manifest. Let us consider a copy of the whole algebra \mathcal{A} , and get the algebra $\mathcal{A} \otimes \mathcal{A}$. The maximally entangled state of two qudits reads

$$|\omega\rangle = \frac{1}{\sqrt{d}} \sum_{j=1}^{d} |jj\rangle$$

This state acts on $\mathcal{A} \otimes \mathcal{A}$ as $\omega(x \otimes y) = \operatorname{tr}(xy^T)$. Then we define the *Choi state* of the QCA α :

$$\phi = (\alpha \otimes \mathbb{1})(\omega).$$

We split the algebra \mathcal{A} at any point n in the lattice:

 $\mathcal{A}_L \equiv \mathcal{A}_{\leq n}$ and $\mathcal{A}_R \equiv \mathcal{A}_{>n}$,

where $\mathcal{A}_{>n} = \{x \in \mathcal{A} \mid x > n\}$ and $\mathcal{A}_{\leq n} = \{x \in \mathcal{A} \mid x \leq n\}$. Similarly $\mathcal{A}_{L'}$ and $\mathcal{A}_{R'}$ are copies of \mathcal{A}_L and \mathcal{A}_R respectively.

The index will be defined in terms of a difference of mutual informations of the Choi state. The mutual information of a state ϕ on $\mathcal{A}_A \otimes \mathcal{A}_B$ is then defined as

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 $I(A:B)_{\phi} = S(\phi, \phi_A \otimes \phi_B)$, where $S(\phi, \phi_A \otimes \phi_B)$ is the relative entropy defined as $S(\phi_A) + S(\phi_B) - S(\phi)$, here S is the Von Neumann entropy. On infinite lattices, relative entropies can be computed as limits, proposition 4.6 of [6]. However, the index will be locally computable.

The index of a QCA α can be calculated as [6]:

$$\operatorname{ind}(\alpha) = \frac{1}{2} \left(I \left(L' : R \right)_{\phi} - I \left(L : R' \right)_{\phi} \right) \,.$$

With this approach it can clearly be seen that the index measures the difference in information flows, left to right minus right to left (figure 3).

As every QCA can be decomposed as shifts and circuits, the validity of this reformulation of the index can be checked by computing it for these two types of QCA.

For a FDQC γ : $|\phi\rangle = U_{LR} \otimes \mathbb{1}_{L'R'} |\omega\rangle_{LL'} |\omega\rangle_{RR'}$. As L and R are entangled with L' and R' respectively and $|\phi\rangle$ is pure: $S(L'_1)_{\phi} = S(L)_{\phi}$, $S(R')_{\phi} = S(R)_{\phi}$ and $S(L'R)_{\phi} = S(LR')_{\phi} \Rightarrow I(L':R)_{\phi} = I(L:R')_{\phi} \Rightarrow$ ind $(\gamma) = 0$. And for a right shift σ , looking at figure 3, it can be seen that I(L:R') = 0, since L and R' are independent, and $I(L':R) = 2\log_2(d)$, since I(L':L) = $S(L) + S(L') + S(LL') = 2S(L) = 2\log_2(d)$ and for the shift R becomes L. Thus, $\operatorname{ind}(\sigma) = \log_2(d)$. For the left shift would be $\operatorname{ind}(\sigma^{-1}) = -\log_2(d)$. These results are the same as at the previous section, as expected.

V. CONCLUSIONS

Quantum cellular automata are a very promising field of research and through this work we have presented a small part of it explaining its fundamental concepts. The equivalence between one-dimensional QCA and matrix product unitaries has been exposed. This allowed us to understand QCA from a tensor network perspective and define an index. This index shows that QCA can be classified according to the amount of net information they propagate in one direction. It has also been seen that any

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QCA is a composition of finite depth circuits and shift operators, which indicates that information flow is only added by shifts.

Very interesting results have recently been published following this line of research. For instance, in [6] it is showed how lattices evolving via time-dependent Hamiltonians satisfying Lieb-Robinson bounds can be understood by QCA approximations. In addition, thanks to the mutual information approach its index can be calculated and shown to be nought, i.e. they cannot implement shifts and propagate net information. On the other hand, in [16] the index theory has been extended to two dimensions, showing that it can fully classify 2D QCA and is deeply related to the topology of the lattice. It is also explained that it seems unlikely a complete classification for higher dimensional QCA can be obtained through the index theorem. Finally, in [17] a physical realization of QCA using lattices of ultracold atoms excited to Rydberg states is proposed.



FIG. 3: Representation of the application of a QCA to the algebra $\mathcal{A} \otimes \mathcal{A}$. The information flows have been represented with dashed lines. The index measures the "net" flow, the difference between the flow from left to right minus right to left.

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