A short introduction to quantum cellular automata and their classification in one and two dimensions

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In this short paper, we will briefly introduce the concepts of quantum cellular automata and how they are classified in one and two dimensions.

INTRODUCTION TO QCA

Recently, people have been discovering that quantum cellular automata (QCA) play an important role in many fields of physics, such as floquet systems [1], topological phases of matter [2], etc.

In this section, we will introduce the setups and define QCA [3, 4] .

Roughly speaking, a QCA is a "unitary evolution" that takes a local operator and its output operator is also local and not far away from the support of the input operator.

Mathematically, we can give the following definition of QCA:

Consider a graph G, with a finite set of vertices (called sites) V. The Hilbert space of the system is a tensor product of finite-dimensional local Hilbert space:

$$\mathcal{H} = \otimes_{i\in V}\mathcal{H}_i, \quad \mathrm{dim}\mathcal{H}_i < \infty.$$

Furthermore, we assume the graph G has a graph metric, i.e. one can compute distance between any two sites, and talk about locality.

Definition 1 *A QCA is an automorphism α of the algebra $\mathcal{A}$ of operators on $\mathcal{H}$:*

$$\alpha(O) = UOU^\dagger, \quad O \in \mathcal{A}, \quad U \textit{ is unitary},$$

subject to the locality-preserving condition: $\forall O_x$ (with $\mathrm{supp}(O_x) = x \in V$), $\alpha(O_x)$ is supported on the sites within distance R from site x. R is called the range of the QCA.

It's possible to generalize the definition in the following ways:

- There might be infinite number of sites. In this case, the automorphism might not be implemented by a mathematically well-defined unitary operator[10].
- The locality-preserving might not be strict, i.e. the support of $\alpha(O_x)$ might be within the distance R up to some quickly-decaying (say exponentially-decaying) error. Hastings called such a case "locally preserving unitary" [5].
- It's possible to generalize it to fermionic system.

Example 1 (Local finite depth quantum circuit) *One can easily think of a class of examples of QCA via finite depth quantum circuit. Since at each layer (step) in the circuit, the unitary operators of the quantum gates have bounded supports, then for a local operator evolved with finite number of such kinds of layers, the support of the resulting operator must still be bounded.*

CLASSIFICATION OF QCA IN ONE AND TWO DIMENSIONS

In this section, we will introduce the classification of QCAs in one and two dimensions [3, 6].

To talk about classification, we first need to define the meaning of equivalence of QCAs:

Definition 2 *For two QCA α, β, they are said to be R-path equivalent if there exists a continuous "path" (i.e. one parameter family) of QCA $\{\alpha_t\}|_{t\in[0,1]}$ of range R, with $\alpha_0 = \alpha, \alpha_1 = \beta$.*

Moreover, such an equivalence relation is said to be "stable" if one tensors identity map to the two ends $\alpha \to \alpha \otimes \mathrm{id}$, $\beta \to \beta \otimes \mathrm{id}$, and it's still R-path equivalent between $\alpha \otimes \mathrm{id}$ and $\beta \otimes \mathrm{id}$. Sometimes, people will drop the word "path".

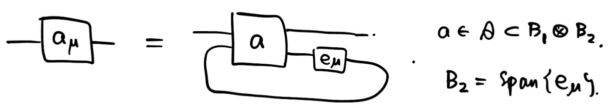
QCA in one dimension

In one dimension, QCA can be classified by an index theory. The construction of the index is as follows:

1. Regroup the sites to obtain a nearest neighbour QCA. This is always achievable. Let $\mathcal{A}_i$ be the algebra of operators on local Hilbert space $\mathcal{H}_i$ associated with the super-site i.
2. Before explicitly define the index, we need to first define a concept called "support algebra":

Definition 3 *Let $\mathcal{A}, \mathcal{B}_1, \mathcal{B}_2$ be algebras with $\mathcal{A} \subset \mathcal{B}_1 \otimes \mathcal{B}_2$. Choose a basis of $\mathcal{B}_2$, say $\{e_\mu\}$ then $\forall a \in \mathcal{A}$, expand it as $a = \sum_\mu a_\mu \otimes e_\mu$. The support algebra $\mathcal{S}(\mathcal{A}, \mathcal{B}_1)$ is spanned by all a_μ's:*

$$\mathcal{S}(\mathcal{A}, \mathcal{B}_1) := \mathrm{Span}\{a_\mu | a = \sum_\mu a_\mu \otimes e_\mu, \forall a \in \mathcal{A}\}. \quad (1)$$



One can see it's actually independent of the choice of the basis $\{e_\mu\}$ of $\mathcal{B}_2$.

3. Let α be the QCA to which we want to put an index. We want to study how algebras $\mathcal{A}_{2n} \otimes \mathcal{A}_{2n+1}$ of $\mathcal{H}_{2n} \otimes \mathcal{H}_{2n+1}$ get evolved by α, where the subscripts are the labels of the super-sites. Therefore, define the following two algebras

$$\mathcal{R}_{2n} = \mathcal{S}(\alpha(\mathcal{A}_{2n} \otimes \mathcal{A}_{2n+1}), \mathcal{A}_{2n-1} \otimes \mathcal{A}_{2n}) \tag{2}$$

$$\mathcal{R}_{2n+1} = \mathcal{S}(\alpha(\mathcal{A}_{2n} \otimes \mathcal{A}_{2n+1}), \mathcal{A}_{2n+1} \otimes \mathcal{A}_{2n+2}) \tag{3}$$

to describe the evolution of $\mathcal{A}_{2n} \otimes \mathcal{A}_{2n+1}$ to the left and to the right respectively. Most importantly, there is a lemma [6] indicates

$$\mathcal{R}_{2n} \otimes \mathcal{R}_{2n+1} = \alpha(\mathcal{A}_{2n} \otimes \mathcal{A}_{2n+1}), \tag{4}$$

which results in

$$\dim(\mathcal{R}_{2n}) \cdot \dim(\mathcal{R}_{2n+1}) = \dim(\mathcal{A}_{2n}) \cdot \dim(\mathcal{A}_{2n+1}), \tag{5}$$

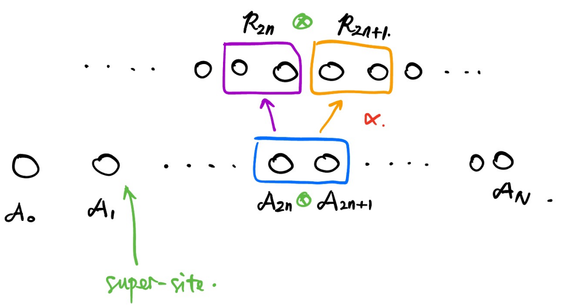
and similarly

$$\dim(\mathcal{R}_{2n+1}) \cdot \dim(\mathcal{R}_{2n+2}) = \dim(\mathcal{A}_{2n+1}) \cdot \dim(\mathcal{A}_{2n+2}). \tag{6}$$

4. Finally, we can define the index (called GNVW index [11]) of α as

$$\mathrm{ind}(\alpha) = \log\left(\sqrt{\frac{\dim(\mathcal{R}_{2n+1})}{\dim(\mathcal{A}_{2n+1})}}\right) \tag{7}$$

A diagrammatic illustration is

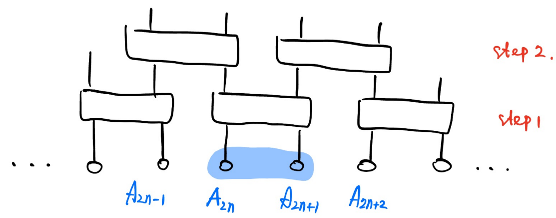


The index has the following properties:

- $e^{\mathrm{ind}(\alpha)}$ are positive rational numbers. This is because both $\mathcal{R}_n$ and $\mathcal{A}_m$ are isomorphic to matrix algebra, whose dimensions are square of integers, say r_n^2, d_m^2 respectively. Therefore, $e^{\mathrm{ind}(\alpha)} = r_{2n+1}/d_{2n+1}$, with $r_{2n+1}, d_{2n+1} \in \mathbb{Z}_+$.
- The index is additive under automorphism composition and tensor products: $\mathrm{ind}(\alpha \cdot \beta) = \mathrm{ind}(\alpha) + \mathrm{ind}(\beta)$, $\mathrm{ind}(\alpha \otimes \beta) = \mathrm{ind}(\alpha) + \mathrm{ind}(\beta)$.
- $\mathrm{ind}(\alpha) = 1$ if and only if α is a finite depth quantum circuit.
- Most importantly, $\mathrm{ind}(\alpha) = \mathrm{ind}(\beta)$ if and only if they are stably equivalent.

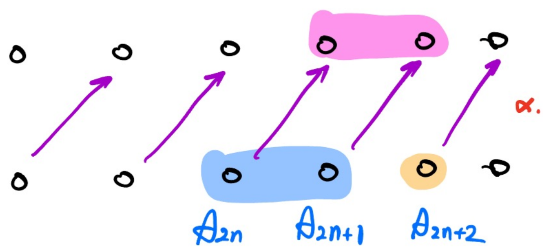
Let's compute the index in the examples of finite depth quantum circuit and shift QCA:

Example 2 (Finite depth quantum circuit) *The following diagram is a depth-2 quantum circuit, where each square is a unitary acting on nearest two sites.*



Consider the resulting support algebras from $\mathcal{A}_{2n} \otimes \mathcal{A}_{2n+1}$, we can see that $\dim(\mathcal{R}_{2n+1}) = \dim(\mathcal{A}_{2n+1})$, therefore $\mathrm{ind}(\alpha) = 0$.

Example 3 (Shift QCA) *Suppose at each site sits a qudit of dimension d, and consider the QCA that shift the support of algebra at m to $m+1$:*



We can see that $\dim(\mathcal{R}_{2n+1}) = d^4, \dim(\mathcal{A}_{2n+1}) = d^2$, therefore $\mathrm{ind}(\alpha) = \log d$.

QCA in two dimensions

The key strategy of classifying QCA in two dimension is by dimensional reduction: Any QCA in two dimension is stably equivalent to some QCA, which agrees with identity everywhere except on some lower dimensional regions [3].

The precise statement is the following:

Theorem 4 *For any QCAs on two dimensional manifold with range $R = O(1)$, each QCA is stably $O(R)$-equivalent to a shift QCA acting on a set of cycles which* *form a basis of the first homology group of the manifold, up to the torsion of the manifold.*

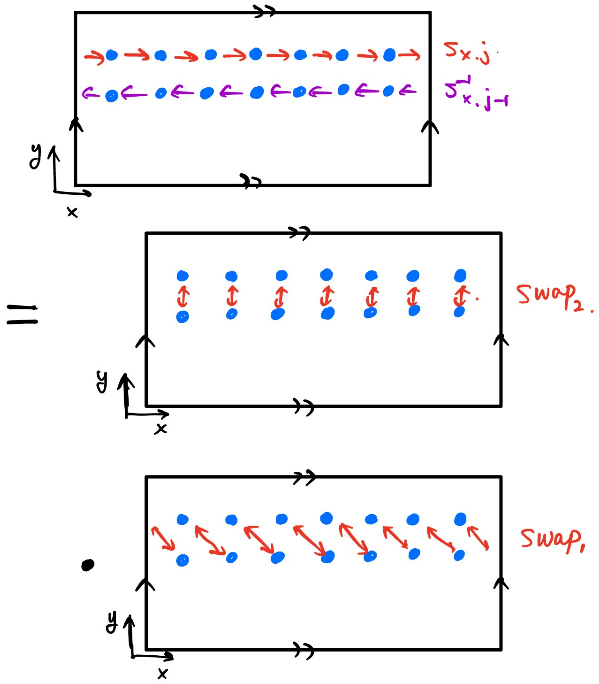
Remarks:

- $O(a)$ means of the same order as a.
- The first homology characterize the non-trivial 1-cycles. If a 1-cycle can be contracted to a point, then it's regarded as trivial.
- Moreover, if the manifold has torsion, one can flip the direction of a 1-cycle. Therefore one might be able to trivialize a pairs of non-trivial 1-cycles.

Therefore, one can reduce the two dimensional QCA to 1-cycles (classified by first homology up to torsion), then use the GNVW index to classify those QCA on 1-cycles.

A detailed proof is beyond the scope of this short paper. We will only demonstrate the idea in the following example of QCA on torus.

Suppose we have two shift QCA in x direction, $s_{x,j}, s_{x,j-1}^{-1}$. One at $y = j$ to the right direction, the other at $y = j - 1$ to the left direction. We can see that $s_{x,j} \cdot s_{x,j-1}^{-1}$ is the same as two swappings $\text{swap}_2 \cdot \text{swap}_1$:



As the composition of two swappings is a finite depth circuit, we can conclude $s_{x,j} \simeq s_{x,j+1}$ up to a finite depth circuit.

By such kind of technique, one can deform a 1-cycle, or move it around, as long as there is no topological obstruction forbidding it. For example, if a 1-cycle encloses a hole, then it cannot be moved to somewhere, or deformed, such that there is no hole enclosed by it. Mathematically, such a property is described by the first homology group of the manifold.

Therefore, we can intuitively see that how to classify 1-cycle (i.e. homology group and torsion of the manifold) should play an important role in classifying QCA.

SUMMARY

In this paper, we briefly introduced the classification of QCA in one and two dimensions. In one dimension, it's classified by GNVW index; and in two dimension, it's classified by the first homology of the manifold up to torsion, together with the GNVW index.

We can see that finite depth quantum circuit and shift QCA play an important role in classifying QCAs in one and two dimensions. However, it's worth pointing out that, there are examples in three dimension [2, 7], which is beyond such a "finite depth circuit plus shift QCA" class. It reminds an interesting question that how the three dimensional QCAs are classified.

What's more, classifying quasi-locality-preserving QCAs is also an intriguing question [8].

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[9] P. Naaijkens, *Quantum Spin Systems on Infinite Lattices* (Springer International Publishing, 2017), URL `https://doi.org/10.1007%2F978-3-319-51458-1`.

[10] For example, consider an infinite spin-1/2 system. Due to the convergence issue, the inner product of $\mathcal{H} \otimes_{i\in\mathbb{Z}} \mathbb{C}^2$,

which seems to be a natural construction of the Hilbert space, is ill-defined. Even if we accept such a $\mathcal{H}$ as a Hilbert space, a multiplication of infinite number of unitaries might not converge. For these mathematical difficulties, people usually consider operator algebras (associated with local observables), and use the word "automorphism" rather than unitary operators. See [9] for an introduction of infinite quantum systems.

[11] We follow the definition in [3]. People also define it without taking the log, as in [1, 6]. Beware in [4], it's inverse to the one used in [1, 6].