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# Generalized Partitioned Quantum Cellular Automata and Quantization of Classical CA

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## Abstract

In this paper, in order to investigate natural transformations from discrete CA to QCA, we introduce a formulation of finite cyclic QCA and generalized notion of partitioned QCA. According to the formulations, we demonstrate the condition of local transition functions, which induce a global transition of well-formed QCA. Following the results, extending a natural correspondence of classical cells and quantum cells to the correspondence of classical CA and QCA, we have the condition of classical CA such that CA generated by quantization of its cells is well-formed QCA. Finally we report some results of computer simulations of quantization of classical CA.

## 1 Introduction

J. Watrous introduced the notion of quantum cellular automata(QCA) and showed that any quantum Turing machine can be efficiently simulated by a QCA with constant slowdown in 1995. C. Dürr and M. Santha [4] considered the properties between local function of quantum cellular automata and the unitarity of the global time evolution operator and proposed an algorithm to decide if a linear quantum cellular automaton is unitary. W. van Dam [14, 15] focused on a quantum cellular automata with circular bounded configurations. He also introduced an periodic quantum gate cellular automata and prove that the universality of it.

CA with quantum cells is well-formed QCA if and only if its global transition function is unitary. Generally quantization of cells of a classical CA dose not always induce a QCA, because usually classical CA dose not have reversibility. Morita and Harao show that we can get reversible CA by partition a cell into three part and partitioned CA can simulate non-partitioned CA[11]. But there is not a trivial inclusion relation between partitioned CA and non-partitioned CA.

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In this paper, we introduce another systematic formulation of finite cyclic QCA and generalized notion of partitioned QCA in order to investigate natural transformation from discrete classical CA to QCA.

According to the formulations, we demonstrate a condition of a local transition function, which induce a well-formed QCA. A natural correspondence of classical cells and quantum cells can be extended to the correspondence of classical CA and QCA. If a classical CA satisfies our conditions then the extended QCA is well-formed. Finally we report some results of computer simulations of quantization of classical CA.

## 2 Preliminaries

Let  $Q$  be a set of states of cells and  $|Q| = s$ . We consider  $Q^n$  is the set of configurations of CA where  $n$  is the size of CA.  $q_i$  denotes the  $i$ th element of the configuration  $q \in Q^n$ , and assume that  $q_0 = q_n$  and  $q_{n+1} = q_1$ .

Before considering computing process of quantum states, we recall that of deterministic states. We use the set of all subset of  $Q$ , that is, the set  $2^Q$  of all functions from  $Q$  to  $2 = \{0, 1\}$  to represent nondeterministic states.

A element  $q$  of  $Q$  is normally considered as an element  $\{q\}$  of  $2^Q$ . Let  $\Sigma$  be the finite set of input characters, then a transition function of input characters of deterministic finite automata is provided as  $\delta : Q \times \Sigma \rightarrow Q$ , and expanded naturally into the transition function  $\delta_* : Q \times \Sigma^* \rightarrow Q$  of input strings. Let  $[\delta] : Q \times \Sigma \rightarrow 2^Q$  be a function defined by  $[\delta](q, \alpha) = [\delta(q, \alpha)]$ .

The function  $[\delta]$  is a state transition function of nondeterministic finite automata and we can expand  $[\delta]$  into  $[\delta]_* : Q \times \Sigma^* \rightarrow 2^Q$ . Recall  $[\delta_*] : Q \times \Sigma^* \rightarrow 2^Q$  be a function defined by  $[\delta_*](q, \alpha) = [\delta_*(q, \alpha)]$ , and we can show that  $[\delta_*] = [\delta]_*$  easily. This shows that the set of all deterministic finite automata are included in the set of all nondeterministic finite automata naturally.

We can consider quantum states as generalized states of classical state and extend to a quantum formulation of computer system. But a classical computer system is not always a quantum computer system generally, because a quantum computing process should be a unitary operator and every classical computing process is not so.

A quantum state denotes a function from a finite set  $Q$  to a set of complex numbers  $\mathbf{C}$  and  $\mathbf{C}^Q$  is denoted by the set of all functions from  $Q$  to  $\mathbf{C}$ . For  $q \in Q$  we define  $[q] \in \mathbf{C}^Q$  as follows;

$$[q](x) = \begin{cases} 1 & (x = q) \\ 0 & (x \neq q) \end{cases}$$

$\mathbf{C}^Q$  is a linear space on  $\mathbf{C}$  such that its bases is  $Q$ . An inner product in  $\mathbf{C}^Q$  is defined by  $\langle p, q \rangle = \sum_{x \in Q} (p(x) \cdot q(x))$  where  $p, q \in \mathbf{C}^Q$ .

A linear space  $\mathbf{C}^{(Q^n)}$  on  $\mathbf{C}$  is considered as a tensor product  $\underbrace{\mathbf{C}^Q \otimes \mathbf{C}^Q \otimes \dots \otimes \mathbf{C}^Q}_n$ , that is, for  $p \in Q^n$   $[p] = [p_1] \otimes [p_2] \otimes \dots \otimes [p_n]$ . For  $p, q \in Q^n$  the inner product

$\langle [p], [q] \rangle$  on  $\mathbf{C}^{(Q^n)}$  is as follows;

$$\begin{aligned}
& \langle [p], [q] \rangle \\
&= \sum_{x \in Q^n} ([p](x) \cdot [q](x)) \\
&= \sum_{(x_1, x_2, \dots, x_n) \in Q^n} (([p_1](x_1)[p_2](x_2) \cdots [p_n](x_n)) \\
&\quad \cdot ([q_1](x_1)[q_2](x_2) \cdots [q_n](x_n))) \\
&= \sum_{x_1 \in Q} ([p_1](x_1)[q_1](x_1)) \cdot \sum_{x_2 \in Q} ([p_2](x_2)[q_2](x_2)) \\
&\quad \cdots \sum_{x_n \in Q} ([p_n](x_n)[q_n](x_n)) \\
&= \langle [p_1], [q_1] \rangle \langle [p_2], [q_2] \rangle \cdots \langle [p_n], [q_n] \rangle.
\end{aligned}$$

For a function  $F : Q^n \rightarrow \mathbf{C}^{(Q^n)}$ , we define functions  $\alpha_F : Q^n \times Q^n \rightarrow \mathbf{C}$  and  $\bar{F} : \mathbf{C}^{(Q^n)} \rightarrow \mathbf{C}^{(Q^n)}$  by  $\alpha_F(p, q) = F(p)(q)$  and  $\bar{F}(X) = \sum_{q \in Q^n} (X(q)(F(q)))$ . We

call  $\bar{F}$  is *unitary* if  $\|\bar{F}(X)\| = 1$  for any  $X \in \mathbf{C}^{(Q^n)}$  such that  $\|X\| = 1$ .

Since  $Q$  is finite, we can label elements of  $Q$  numbers from 1 to  $s$  and also elements of  $Q^n$  numbers from 1 to  $s^n$  by lexicographical ordering. We define a  $s^n \times s^n$  matrix  $(\alpha_{ij})$  by  $\alpha_{ij} = \alpha_F(p, q)$  where numbers of elements  $p$  and  $q$  are  $i$  and  $j$ .

**Proposition 1** *If the matrix  $(\alpha_{i,j})$  is unitary then  $\bar{F}$  is unitary.*

**Proof.** Assume that  $(\alpha_{ij})$  is a unitary matrix and  $\langle X, X \rangle = 1$ .

$$\begin{aligned}
& \langle \bar{F}(X), \bar{F}(X) \rangle \\
&= \langle \sum_{p \in Q^n} X(p)\bar{F}(p), \sum_{q \in Q^n} X(q)\bar{F}(q) \rangle \\
&= \sum_{p \in Q^n} \sum_{q \in Q^n} \langle X(p)\bar{F}(p), X(q)\bar{F}(q) \rangle \\
&= \sum_{p \in Q^n} (X(p) \sum_{q \in Q^n} (X(q) \sum_{r \in Q^n} (\bar{F}(p)(r) \cdot \bar{F}(q)(r)))) \\
&= \sum_{p \in Q^n} (X(p) \sum_{q \in Q^n} (X(q) \sum_{r \in Q^n} (\alpha(p, r) \cdot \alpha(q, r)))) \\
&= \sum_{p \in Q^n} (X(p) \sum_{q \in Q^n} (X(q) \sum_{r \in Q^n} (\alpha(p, r) \cdot \overline{\alpha(r, q)}))) \\
&= \sum_{p \in Q^n} (X(p) \cdot X(p)) \\
&= 1
\end{aligned}$$

So  $\bar{F}$  is unitary. □

**Proposition 2** Let  $\hat{\sigma} : \mathbf{C}^{Q^n} \rightarrow \mathbf{C}^{Q^n}$  be defined by  $\hat{\sigma}(X) = \sum_{p \in Q^n} (X(p)[\sigma(p)])$  where  $\sigma : Q^n \rightarrow Q^n$ . Then  $\hat{\sigma}$  are unitary if and only if  $\sigma$  is a bijection.

**Proof.** (If) Assume that  $\sigma$  is bijection and  $\langle X, X \rangle = 1$ .

$$\begin{aligned}
& \langle \hat{\sigma}(X), \hat{\sigma}(X) \rangle \\
&= \sum_{p \in Q^n} (\hat{\sigma}(X)(p), \hat{\sigma}(X)(p)) \\
&= \sum_{p \in Q^n} \left( \sum_{q \in Q^n} (X(q)[\sigma(q)](p)), \sum_{q \in Q^n} (X(q)[\sigma(q)](p)) \right) \\
&= \sum_{p \in Q^n} (X(\sigma^{-1}(p)), X(\sigma^{-1}(p))) \\
&= \sum_{p \in Q^n} (X(p), X(p)) \\
&= 1
\end{aligned}$$

So  $\hat{\sigma}$  is unitary.

(Only if) Assume that  $\hat{\sigma}$  is unitary and  $\sigma$  is not bijection. Now we let

$$Q_0 = \{q_0 \in Q^n \mid \sigma(p) \neq q_0 \text{ for } \forall p \in Q^n\},$$

$$Q_1 = \{q_1 \in Q^n \mid \exists! p \in Q^n \text{ such that } \sigma(p) = q_1\},$$

$$Q_2 = \{q_2 \in Q^n \mid \exists p_1, p_2 \in Q^n \text{ such that } q_2 = \sigma(p_1) = \sigma(p_2) \text{ and } p_1 \neq p_2\},$$

$|Q_2| = s (\neq 0)$  and

$$X(q) = \begin{cases} \frac{1}{\sqrt{s}} & (q \in Q_2) \\ 0 & \text{otherwise.} \end{cases}$$

Then  $\langle X, X \rangle = 1$  and

$$\begin{aligned}
& \langle \hat{\sigma}(X), \hat{\sigma}(X) \rangle \\
&= \sum_{q \in Q^n} (\hat{\sigma}(X)(q) \cdot \hat{\sigma}(X)(q)) \\
&= \sum_{q \in Q^n} \left( \sum_{p \in Q^n} (X(p)[\sigma(p)](q)) \cdot \sum_{p \in Q^n} (X(p)[\sigma(p)](q)) \right) \\
&= \sum_{q \in Q^n} \left( \sum_{\sigma(p)=q} X(p) \cdot \sum_{\sigma(p)=q} X(p) \right) \\
&= \sum_{q \in Q_2} \left( \sum_{\sigma(p)=q} X(p) \cdot \sum_{\sigma(p)=q} X(p) \right) \\
&\neq 1
\end{aligned}$$

This is contradiction. So we get that  $\sigma$  is bijection.  $\square$

A classical CA[17] is a transition system in  $Q$  defined by a global transition function  $F : Q^n \rightarrow Q^n$  where  $F(q)_i = f(q_{i-1}, q_i, q_{i+1})$  and  $f : Q \times Q \times Q \rightarrow Q$  is a local transition function.

When  $Q = \{0, 1\}$ , a local transition function is defined by the eight values  $f(0, 0, 0) = r_0$ ,  $f(0, 0, 1) = r_1$ ,  $f(0, 1, 0) = r_2$ ,  $f(0, 1, 1) = r_3$ ,  $f(1, 0, 0) = r_4$ ,  $f(1, 0, 1) = r_5$ ,  $f(1, 1, 0) = r_6$  and  $f(1, 1, 1) = r_7$  ( $r_i = 0, 1$ ). The rule number  $R$  of a local transition function  $f$  is defined by

$$R = 2^7 r_7 + 2^6 r_6 + 2^5 r_5 + 2^4 r_4 + 2^3 r_3 + 2^2 r_2 + 2^1 r_1 + r_0.$$

The local transition function of rule number  $R$  is denoted by  $f_R$ . The local transition rules with rule number 204, 240 and 170 are illustrated as follows;

204	111	110	101	100	011	010	001	000
	1	1	0	0	1	1	0	0
240	111	110	101	100	011	010	001	000
	1	1	1	1	0	0	0	0
170	111	110	101	100	011	010	001	000
	1	0	1	0	1	0	1	0

$f_{204}$ ,  $f_{240}$  and  $f_{170}$  are identity, shift-right and shift-left functions respectively.

### 3 Quantum Cellular Automata

The global transition function  $F : Q^n \rightarrow \mathbf{C}^{(Q^n)}$  is defined by  $F_h(q)(x) = h(q_0, q_1, q_2)(x_1) \cdot h(q_1, q_2, q_3)(x_2) \cdots h(q_{n-1}, q_n, q_{n+1})(x_n)$  for a local transition function  $h : Q \times Q \times Q \rightarrow \mathbf{C}^Q$ . A transition system in  $\mathbf{C}^{(Q^n)}$  is defined by  $\overline{F_h} : \mathbf{C}^{(Q^n)} \rightarrow \mathbf{C}^{(Q^n)}$ . The local transition function  $h$  is called 'forming a quantum cellular automaton' if  $\overline{F_h}$  is unitary.

Let  $F_f : Q^n \rightarrow Q^n$  be a global transition function of a local transition function  $f : Q^3 \rightarrow Q$ , and  $[F_f] : Q^n \rightarrow \mathbf{C}^{Q^n}$  a function such that  $[F_f](x) = [F_f(x)]$  for  $x \in Q^n$ . And we let  $[f] : Q^3 \rightarrow \mathbf{C}^Q$  be a local transition function of QCA such that  $[f](x) = [f(x)]$  for  $x \in Q^3$ , and  $F_{[f]} : Q^n \rightarrow \mathbf{C}^{(Q^n)}$  its global transition function. Then we can show that  $[F_f] = F_{[f]}$  by easy computation. But a local transition functions  $[f] : Q^3 \rightarrow \mathbf{C}^Q$  does not always form a QCA, that is, a  $\overline{[F_f]}$  is not always unitary. W. van Dam[14, 15] introduced a formulation of cyclic quantum cellular automata and investigate their properties of well-formedness. We focused on reinvestigating similar results related with the extension of classical CA and their local functions.

**Proposition 3**  $[f]$  is forming a quantum cellular automata if and only if  $F_f : Q^n \rightarrow Q^n$  is a bijection.

**Proof.** For  $X \in \mathbf{C}^{(Q^n)}$

$$\begin{aligned} \overline{F_{[f]}}(X) &= \overline{[F_f]}(X) \\ &= \sum_{q \in Q^n} (X(q)([F_f](q))) \\ &= \sum_{q \in Q^n} (X(q)([F_f(q)])) \\ &= \hat{F}_f(X). \end{aligned}$$

So this is derived from proposition 2.  $\square$

## 4 Partitioned Quantum Cellular Automata

We define functions  $G : Q^n \rightarrow \mathbf{C}^{(Q^n)}$  and  $\lambda : Q \times Q \rightarrow \mathbf{C}$  by  $G(q)(x) = g(q_1)(x_1) \cdot g(q_2)(x_2) \cdots g(q_n)(x_n)$  and  $\lambda(p, q) = g(p)(q)$  for a function  $g : Q \rightarrow \mathbf{C}^Q$ .

We label the elements of  $Q^n$  numbers from 1 to  $s^n$  and define a  $s^n \times s^n$  matrix  $(\alpha_{ij})$  from  $\alpha_G : Q^n \times Q^n \rightarrow \mathbf{C}$ . And we label the elements of  $Q$  numbers from 1 to  $s$  and define a  $s \times s$  matrix  $(\lambda_{ij})$  from the function  $\lambda$ .

**Proposition 4**  $(\lambda_{ij})$  is a unitary matrix if and only if  $(\alpha_{ij})$  is a unitary matrix.

**Proof.** (Only if) Assume that  $(\lambda_{i,j})$  is unitary.

$$\begin{aligned}
& \sum_{q \in Q^n} (\alpha(p, q) \cdot \alpha(r, q)) \\
&= \sum_{q \in Q^n} (G(p)(q) \cdot G(r)(q)) \\
&= \sum_{q_1 \in Q} \cdots \sum_{q_n \in Q} g(p_1)(q_1) \cdots g(p_n)(q_n) \cdot g(r_1)(q_1) \cdots g(r_n)(q_n) \\
&= \lambda(p_1, r_1) \cdot \lambda(p_2, r_2) \cdots \lambda(p_n, r_n) \\
&= \langle [p_1], [r_1] \rangle \cdot \langle [p_2], [r_2] \rangle \cdots \langle [p_n], [r_n] \rangle \\
&= \langle [p], [r] \rangle
\end{aligned}$$

So  $\alpha_{i,j}$  is unitary.

(If) Assume that  $\alpha_{i,j}$  is unitary and  $\lambda_{i,j}$  is not so, that is,  $\lambda(p_i, q_i) \neq \langle [p_i], [q_i] \rangle$ .

Then

$$\begin{aligned}
\sum_{q \in Q^n} (\alpha(p, q) \cdot \alpha(r, q)) &= \lambda(p_1, r_1) \cdot \lambda(p_2, r_2) \cdots \lambda(p_n, r_n) \\
&\neq \langle [p_1], [r_1] \rangle \cdot \langle [p_2], [r_2] \rangle \cdots \langle [p_n], [r_n] \rangle \\
&= \langle [p], [r] \rangle
\end{aligned}$$

This is contradiction. So  $\lambda_{i,j}$  is unitary.  $\square$

**Proposition 5** If  $\sigma : Q^n \rightarrow Q^n$  is a bijection, then the followings hold;

(i)  $\overline{G \circ \sigma} = \overline{G} \circ \hat{\sigma}$ .

(ii)  $\overline{G \circ \sigma}$  is unitary if and only if  $\overline{G}$  is unitary.

$$\begin{array}{ccccc}
Q^n & \xrightarrow{\sigma} & Q^n & \xrightarrow{G} & \mathbf{C}^{(Q^n)} \\
\downarrow & & \downarrow & & \updownarrow \\
\mathbf{C}^{(Q^n)} & \xrightarrow{\hat{\sigma}} & \mathbf{C}^{(Q^n)} & \xrightarrow{\overline{G}} & \mathbf{C}^{(Q^n)}
\end{array}$$

**Proof.**



(i)

$$\begin{aligned}
\overline{G \circ \sigma}(X) &= \sum_{q \in Q^n} (X(q)((G \circ \sigma)(q))) \\
&= \sum_{q \in Q^n} (X(q)(G(\sigma(q)))) \\
&= \sum_{p \in Q^n} (X(\sigma^{-1}(p))(G(q))) \\
&= \sum_{p \in Q^n} ((\sum_{r \in Q^n} (X(r)[\sigma(r)]))(q)(G(q))) \\
&= \sum_{p \in Q^n} (\hat{\sigma}(X)(q)(G(q))) \\
&= \overline{G} \circ \hat{\sigma}(X)
\end{aligned}$$

(ii) (If) It is trivial from (i) and proposition 2.

(Only if) Assume that  $\overline{G \circ \sigma} = \overline{G} \circ \hat{\sigma}$  is unitary and  $\overline{G}$  is not so, that is,  $\langle \overline{G \circ \sigma}(X), \overline{G \circ \sigma}(X) \rangle = 1$  and  $\langle \hat{\sigma}(X), \hat{\sigma}(X) \rangle = 1$  for any  $X \in \mathbf{C}^{(Q^n)}$  such that  $\langle X, X \rangle = 1$ , and there exists  $Y \in \mathbf{C}^{(Q^n)}$  such that  $\langle Y, Y \rangle = 1$  and  $\langle \overline{G}(Y), \overline{G}(Y) \rangle \neq 1$ . Then

$$\begin{aligned}
1 &= \langle \overline{G \circ \sigma}(\hat{\sigma}^{-1}(Y)), \overline{G \circ \sigma}(\hat{\sigma}^{-1}(Y)) \rangle \\
&= \langle \overline{G} \circ \hat{\sigma}(\hat{\sigma}^{-1}(Y)), \overline{G} \circ \hat{\sigma}(\hat{\sigma}^{-1}(Y)) \rangle \\
&= \langle \overline{G}(\hat{\sigma}(\hat{\sigma}^{-1}(Y))), \overline{G}(\hat{\sigma}(\hat{\sigma}^{-1}(Y))) \rangle \\
&= \langle \overline{G}(Y), \overline{G}(Y) \rangle \\
&\neq 1
\end{aligned}$$

□

**Theorem 6** *The composition function  $f = g \circ e : Q^3 \rightarrow \mathbf{C}^Q$  of functions  $e : Q^3 \rightarrow Q$  and  $g : Q \rightarrow \mathbf{C}^Q$  is forming a quantum cellular automaton if both of the following two conditions hold:*

(i)  $F_e : Q^n \rightarrow Q^n$  is a bijection.

(ii) The matrix  $(\lambda_{ij})$  defined from  $g : Q \rightarrow \mathbf{C}^Q$  is unitary.

**Proof.** At First we show that  $\overline{F_f} = \overline{G} \circ \overline{F_e}$ .

$$\begin{aligned}
&G \circ F_e(q)(x) \\
&= g(e(q_0, q_1, q_2))(x_1) \cdot g(e(q_1, q_2, q_3))(x_2) \cdots g(e(q_{n-1}, q_n, q_{n+1}))(x_n) \\
&= (g \circ e)(q_0, q_1, q_2)(x_1) \cdot (g \circ e)(q_1, q_2, q_3)(x_2) \cdots (g \circ e)(q_{n-1}, q_n, q_{n+1})(x_n) \\
&= F_{g \circ e}(q)(x).
\end{aligned}$$

Therefore

$$\begin{aligned}
\overline{F_f}(X) &= \overline{F_{g \circ e}}(X) \\
&= \sum_{q \in Q^n} (X(q)(F_{g \circ e}(q))) \\
&= \sum_{q \in Q^n} (X(q)(G \circ F_e)(q)) \\
&= \overline{G \circ F_e}(X).
\end{aligned}$$

So we can prove this by proposition 4 and 5.  $\square$

**Example 7** Let  $Q = L \times M \times R$  for finite sets  $L$ ,  $M$  and  $R$ . We define  $e : Q^3 \rightarrow Q$  and  $g : Q \rightarrow \mathbf{C}^Q$  by  $e(((l_1, m_1, r_1), (l_2, m_2, r_2), (l_3, m_3, r_3))) = (l_3, m_2, r_1)$  and  $g(q) = [q]$ . Then the composition function  $f = g \circ e$  is forming a quantum cellular automaton. Because  $F_e : Q^n \rightarrow Q^n$  is a bijection,  $F_e(((l_i, m_i, r_i)))_j = (l_{j+1}, m_j, r_{j-1})$ , and  $(\lambda_{ij})$  defined from  $g$  is an identity matrix.

In example 7, we can replace  $g$  to another function  $g : Q \rightarrow \mathbf{C}^Q$  where the matrix  $(\lambda_{ij})$  defined from  $g$  is unitary. On that occasion  $f : (L \times M \times R)^3 \rightarrow (L \times M \times R)$  is also forming a quantum cellular automaton. Consequently a partitioned quantum cellular automaton introduced in [16] is demonstrated as a special case of our general formulation.

**Example 8** Let  $Q = \{0, 1\}$ ,  $e : Q^3 \rightarrow Q$  be a function such that  $F_e : Q^n \rightarrow Q^n$  is a bijection, and  $\Lambda = (\lambda_{ij})$  defined from  $g : Q \rightarrow \mathbf{C}^Q$  be as follows;

$$\Lambda = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}.$$

Then the local transition function defined from  $f = g \circ e$  forms a quantum cellular automaton. This shows a quantum cellular automaton formed by a synthesised function of a local transition function  $e$  and its reverse function. That is, if  $\theta = 0$  then  $f = e$  and if  $\theta = \frac{\pi}{2}$  then  $f$  is the reversed function of  $e$ , so we can consider  $f$  for  $0 < \theta < \frac{\pi}{2}$  as a synthesised function of two classical local functions.

**Example 9** Let  $Q = \{0, 1\} \times \{0, 1\}$ ,  $e((a_1, b_1), (a_2, b_2), (a_3, b_3)) = (a_1, b_3)$ , and  $\Lambda = (\lambda_{ij})$  defined by  $g : Q \rightarrow \mathbf{C}^Q$  be as follows;

$$\Lambda = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Then  $f = g \circ e$  forms a QCA and  $f((a_1, b_1), (a_2, b_2), (a_3, b_3)) = (a_1, a_1 \oplus b_3)$ .

## 5 Computer Analysis

The following is a table of the size  $n$  of CA and rule number  $R$  where the local transition function  $f_R : Q^3 \rightarrow Q$  forms QCA ( $Q = \{0, 1\}$ ,  $3 \leq n \leq 22$  and  $128 \leq R \leq 255$ ). We note that if  $f_R$  forms QCA then  $f_{255-R}$  also forms QCA.

Size $n$	Rule number $R$
3	142, 154, 156, 166, 170, 172, 178, 180, 184 198, 202, 204, 210, 212, 216, 226, 228, 240
4, 8, 10, 14 16, 20, 22	150, 170, 204, 240
5, 7, 11, 13, 19	150, 154, 166, 170, 180, 204, 210, 240
9, 15, 21	154, 166, 170, 180, 204, 210, 240
6, 12, 18	170, 204, 240

In the case of size 6, 12 and 18, trivial transitions, that is, identity, right shift and left shift functions only form QCA. In other case, there is a nontrivial transition function forming QCA.

From the above table, we can guess the following table of sizes of CA and rule numbers of local transition functions forming QCA, but we have not proved it yet.

Size ( $k \geq 1$ )	Rule number
$6k \pm 2$	150, 170, 204, 240
$6k \pm 1$	150, 154, 166, 170, 180, 204, 210, 240
$6k + 3$	154, 166, 170, 180, 204, 210, 240
$6k$	170, 204, 240

**Example 10** When the size of CA is 4 or 5, the local transition function  $f_{150}(x, y, z) = x + y + z \pmod{2}$  forms a quantum CA.

Let  $F_f$  be the global transition function, then the following hold;

$$\begin{aligned}
 F_f(x)_i &= x_{i-1} + x_i + x_{i+1} \\
 F_f^2(x)_i &= x_{i-2} + x_{i-1} + x_i \\
 &\quad + x_{i-1} + x_i + x_{i+1} \\
 &\quad + x_i + x_{i+1} + x_{i+2} \\
 &= x_{i-2} + x_i + x_{i+2} \\
 F_f^3(x)_i &= x_{i-3} + x_{i-2} + x_{i-1} \\
 &\quad + x_{i-1} + x_i + x_{i+1} \\
 &\quad + x_{i+1} + x_{i+2} + x_{i+3} \\
 &= x_{i-3} + x_{i-2} + x_i + x_{i+2} + x_{i+3}
 \end{aligned}$$

In the case that the size of CA is 4,  $F_f^2(x)_i = x_{i+2} + x_i + x_{i+2} = x_i$ . So  $F_f^2(x) = x$ . In the case that the size of CA is 5,  $F_f^3(x)_i = x_{i+2} + x_{i+3} + x_i + x_{i+2} + x_{i+3} = x_i$ . So  $F_f^3(x) = x$ . Namely there exists  $y$  such that  $F_f(y) = x$  for any  $x \in Q^n$  ( $n = 4, 5$ ), and  $F_f$  is a bijection. So  $f$  forms a QCA.

## 6 Related Works and Conclusion

Cellular automata dealt in this paper is finite cyclic CA and different from CA without boundary, that is, infinite CA dealt by Watrous[16], Morita and Harao[11]. Because the size of CA is finite it does not have the universal computability[12, 1, 2]. But the conditions of local transition functions forming QCA is formulated clearly in our framework.

Injectivity of global maps of classical CA is an essential property for extending to a QCA. The injectivity are considered in [8, 9, 10, 12] for classical CA without boundary and in [6, 3, 7] for classical finite cyclic CA.

A further direction of this study will be to consider properties on construction and synthesis of general quantum computer system by examining construction and synthesis of local transition function of realizable QCA.

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