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# On reversibility of cellular automata with periodic boundary conditions

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#### Abstract

Reversibility of one-dimensional cellular automata with periodic boundary conditions is discussed. It is shown that there exist exactly 16 reversible elementary cellular automaton rules for infinitely many cell sizes by means of a correspondence between elementary cellular automaton and the de Bruijn graph. In addition, a sufficient condition for reversibility of three-valued and two-neighbour cellular automaton is given.

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# 1. Introduction

For the last decade there has been an increasing interest in the study of ultradiscrete dynamical systems, which take discrete values in discrete time steps, from the viewpoint of integrability. In this context, one of the most interesting reversible systems is the box–ball system [1, 2], which is a kind of 'filter' cellular automata. The box–ball systems are an extension of a soliton cellular automaton proposed by Takahashi and Satsuma [3]. These cellular automata have solitonical nature and are directly connected with soliton equations by a procedure called the ultradiscretization [4]. Moreover, they preserve integrable properties such as sufficiently many conserved quantities [5], therefore the box–ball systems are considered to be integrable cellular automata. Imposing periodic boundary conditions to the box–ball systems, their integrability is still preserved [6, 7]. Thus, these integrable cellular automata are considered to be an ultimate discretization of integrable systems and to have rich mathematical structures [8, 9]. On the other hand, although there exist many integrable continuous or discrete systems other than soliton equations, integrable cellular automata other than the box–ball systems are scarcely known. In general, reversibility of a dynamical system is a necessary condition for its integrability, hence if an integrable cellular automaton exists then it must be reversible.

Therefore, if we want to find integrable cellular automata then we have to search reversible ones.

One-dimensional cellular automaton is a discrete dynamical system which is composed of regular array of cells. Each cell takes only a finite number of states which are updated by a local transition function in discrete time steps. The updating rule is quite simple, but cellular automata in general show complicated behaviour [10–12]. Since time evolution of a cellular automaton with periodic boundary conditions can be regarded as a mapping from a finite set into itself, if the mapping is injective then the rule is reversible, that is, the inverse time evolution is uniquely determined. A reversible cellular automaton preserves all information of the initial states in any time step, hence its reversibility suggests existence of conserved quantities. Although reversibility of cellular automata has been discussed many times from various viewpoints [13], as far as the authors know, reversibility of concrete cellular automata rules with periodic boundary conditions for infinitely many cell sizes has not been proved yet except for some cases [14].

In this paper, we show a correspondence between configurations of a cellular automaton with periodic boundary conditions and closed walks in the de Bruijn graph. Using the correspondence, we give a necessary and sufficient condition for reversibility of a cellular automaton rule for infinitely many cell sizes upon the trace of the weighted adjacency matrix of the de Bruijn graph. Then we show reversibility of the rule 154 of elementary cellular automaton. In addition, we show all the reversible elementary cellular automaton rules are the rules 150, 154, 170 and 204 up to automorphisms. We also give a sufficient condition for reversibility of three-valued and two-neighbour cellular automaton for infinitely many cell sizes.

This paper is organized as follows. In section 2, we show a correspondence between configurations of the cellular automaton  $\mathcal{A}_{l}^{(r)}$  with periodic boundary conditions and closed walks in the de Bruijn graph  $G_{l-1}^{(r)}$  through a mapping on the edge set of the graph, and give a necessary and sufficient condition for reversibility of the cellular automaton. In section 3, we classify reversible elementary cellular automaton rules and give the cell sizes for which the rules are reversible. In section 4, we show a sufficient condition for reversibility of the cellular automaton  $\mathcal{A}_{2}^{(3)}$ . Section 5 is devoted to concluding remarks.

# 2. Cellular automata and the de Bruijn graphs

The de Bruijn graph denoted by  $G_l^{(r)}$  can be described as follows. The vertices of  $G_l^{(r)}$  are all the *l*-tuples  $\alpha_1 \alpha_2 \cdots \alpha_l$  where the  $\alpha_i$  range over the elements of  $\mathbb{Z}_r := \{0, 1, 2, \dots, r-1\}$ . A directed edge joins a vertex  $\alpha_1 \alpha_2 \cdots \alpha_l$  to another vertex  $\alpha_2 \alpha_3 \cdots \alpha_l \beta$  and is denoted by  $\alpha_1 \alpha_2 \cdots \alpha_l \beta$ . Hence each vertex of  $G_l^{(r)}$  has both its in-degree and out-degree equal to *r*. The de Bruijn graph  $G_l^{(r)}$  has a unique path of length *l* which connects arbitrary two vertices and  $r^L$  closed walks of length *L* for  $\forall L > l$  [15]. A walk of length *L* in a graph whose first and last edges are *u* and *v*, respectively, is denoted by a sequence of *L* edges as

$$\underbrace{u\cdots v}_{L}$$
.

An example of the de Bruijn graph,  $G_2^{(2)}$ , is given in figure 1.

There exist graph automorphisms  $\varrho_i$ , i = 1, 2, ..., r - 1 of the de Bruijn graph  $G_l^{(r)}$  given by

$$\varrho_i(\alpha_1\alpha_2\cdots\alpha_{l+1}) = (\alpha_1+i)(\alpha_2+i)\cdots(\alpha_{l+1}+i) \pmod{r}$$



**Figure 1.** The de Bruijn graph  $G_2^{(2)}$ .



**Figure 2.** Time evolution of the ECA rule whose local transition function is (1) for the initial state in which the values of cells are chosen randomly 0 or 1. The number of cells is 301. Cells with value 1 and 0 are shown in black and white respectively. The configurations at successive time steps are shown on successive lines.

where  $\alpha_1 \alpha_2 \cdots \alpha_{l+1}$  is an edge. For the de Bruijn graph  $G_2^{(2)}$ ,  $\varrho_1$  is as follows:  $\varrho_1(111) = 000$   $\varrho_1(110) = 001$   $\varrho_1(101) = 010$   $\varrho_1(100) = 011$   $\varrho_1(011) = 100$   $\varrho_1(010) = 101$   $\varrho_1(001) = 110$   $\varrho_1(000) = 111$ and is realized as the rotation of  $\pi$  in figure 1.

On the other hand, the one-dimensional cellular automaton  $\mathcal{A} = \langle N, \mathbb{Z}_q, E, \delta \rangle$  is defined by the one-dimensional array of N cells, a finite set of values  $\mathbb{Z}_q$ , the neighbourhood

by the one-dimensional array of N cells, a finite set of values  $\mathbb{Z}_q$ , the neighbourhood  $E := \{e_1, e_2, \ldots, e_k\}$  and a local transition function  $\delta : \mathbb{Z}_q^k \to \mathbb{Z}_q$ . A mapping  $c : \mathbb{Z}_N \to \mathbb{Z}_q$  is called a configuration of  $\mathcal{A}$ . The global transition function  $F_{\mathcal{A}}$  maps the set  $\mathbb{Z}_q^N$  of all the configurations of  $\mathcal{A}$  into itself and is defined by

$$F_{\mathcal{A}}(c) = c'$$

where

$$c'(i) = \delta(c(i+e_1), c(i+e_2), \dots, c(i+e_k))$$
  $i = 1, 2, \dots, N$ 

and  $c(i) \in \mathbb{Z}_q$  stands for the value of the *i*th cell. From now on, a cellular automaton will be assumed to be with periodic boundary conditions, unless otherwise stated. For example, let q = 2 and  $E = \{-1, 0, 1\}$ , then we obtain elementary cellular automaton (ECA)  $\mathcal{A} = \langle N, \mathbb{Z}_2, \{-1, 0, 1\}, \delta_{\text{ECA}} \rangle$ , where  $\delta_{\text{ECA}} : \mathbb{Z}_2^3 \to \mathbb{Z}_2$  is the local transition function. Time evolution of an ECA rule whose local transition function is given as

is shown in figure 2.

We consider two automorphisms on the cellular automaton  $\mathcal{A} = \langle N, \mathbb{Z}_q, E, \delta \rangle$ . One is the reflection  $\sigma$ , which is given by

$$\sigma: \delta(c(i+e_1), c(i+e_2), \dots, c(i+e_k)) \mapsto \delta(c(i+e_k), c(i+e_{k-1}), \dots, c(i+e_1))$$
$$i = 1, 2, \dots, N.$$

By definition,  $\sigma$  satisfies  $\sigma^2 = id$ , that is,  $\sigma$  constitutes the symmetric group  $S_2$  of degree 2. Another is the conjugation  $\tau_j$ , j = 1, 2, ..., p(q) - 1, where q is the number of the elements of  $\mathbb{Z}_q$  and p(q) is the number of partitions of q. The conjugation  $\tau_j$  are induced by the symmetric group  $S_q$  of degree q which acts on  $\mathbb{Z}_q$  and whose element is also denoted by  $\tau_j$ . Each  $\tau_j$  acts on  $\mathcal{A} = \langle N, \mathbb{Z}_q, E, \delta \rangle$  as follows:

 $\tau_j : \delta(c(i+e_1), c(i+e_2), \dots, c(i+e_k))$ 

$$\mapsto \tau_j^{-1}[\delta(\tau_j(c(i+e_1)), \tau_j(c(i+e_2)), \dots, \tau_j(c(i+e_k)))] \qquad i=1, 2, \dots, N.$$

If we put the neighbourhood  $E = \{e_1, e_2, \ldots, e_k\}$  as

$$e_i = e_1 + i - 1$$
  $i = 2, 3, \dots, k$ 

and assume k = l + 1 and q = r then each element of the set of the neighbours  $\mathbb{Z}_q^k = \mathbb{Z}_r^{l+1}$ corresponds to an edge of the de Bruijn graph  $G_l^{(r)}$ . Therefore, it is equivalent to give a mapping  $\phi : \mathcal{E} \simeq \mathbb{Z}_r^{l+1} \to \mathbb{Z}_r$ , where  $\mathcal{E}$  is the edge set of  $G_l^{(r)}$ , and to give a local transition function  $\delta : \mathbb{Z}_r^{l+1} \to \mathbb{Z}_r$  of the cellular automaton  $\mathcal{A}$ . Thus we can identify the mapping  $\phi : \mathcal{E} \to \mathbb{Z}_r$  and a rule of  $\mathcal{A}$ . We call a mapping  $\phi$  identified with the rule R of  $\mathcal{A}$  'the mapping associated with the rule R of  $\mathcal{A}$ ', and denote it by  $\phi_R$ . Hereafter, under the above assumption, the cellular automaton  $\mathcal{A}$  is denoted by  $\mathcal{A}_{l+1}^{(r)}$ .

By the mapping  $\phi_R : \mathcal{E} \to \mathbb{Z}_r$ , each closed walk in  $G_l^{(r)}$  corresponds to a configuration of  $\mathcal{A}_{l+1}^{(r)}$  with periodic boundary conditions as follows [16, 17]. Consider the  $\mathbb{Z}$ -module generated by the edge set  $\mathcal{E}$  of the de Bruijn graph  $G_l^{(r)}$  and denote it also by  $\mathcal{E}$ . Then we regard a closed walk  $\varepsilon_{i_1}\varepsilon_{i_2}\cdots\varepsilon_{i_n}$  in  $G_l^{(r)}$  as an element  $\varepsilon_{i_1}\varepsilon_{i_2}\cdots\varepsilon_{i_n}$  of the tensor product space  $\mathcal{E}^{\otimes n} := \mathcal{E} \otimes \mathcal{E} \otimes \cdots \otimes \mathcal{E}$ . Similarly, we denote the  $\mathbb{Z}$ -module generated by  $\mathbb{Z}_r$  also by

 $\mathbb{Z}_r$  and identify a configuration  $q_{i_1}q_{i_2}\cdots q_{i_n}$  of the cellular automaton  $\mathcal{A}_{l+1}^{(r)}$  and an element  $q_{i_1}q_{i_2}\cdots q_{i_n}$  of  $\mathbb{Z}_r^{\otimes n} := \underbrace{\mathbb{Z}_r \otimes \mathbb{Z}_r \otimes \cdots \otimes \mathbb{Z}_r}$ . Then  $\phi_R^{\otimes N} : \mathcal{E}^{\otimes N} \to \mathbb{Z}_r^{\otimes N}, \phi_R^{\otimes N}(\varepsilon_{i_1}\varepsilon_{i_2}\cdots\varepsilon_{i_N}) :=$ 

 $\phi_R(\varepsilon_{i_1})\phi_R(\varepsilon_{i_2})\cdots\phi_R(\varepsilon_{i_N})$  maps a closed walk of length *N* in  $G_l^{(r)}$  into an element of  $\mathbb{Z}_r^N$ . If the mapping  $\phi_R^{\otimes N}$  is injective then the corresponding rule is reversible for the cell size *N*. Because the number of possible configurations of  $\mathcal{A}_{l+1}^{(r)}$  is  $q^N = r^N$  and  $G_l^{(r)}$  has  $r^N$  closed walks of length *N* for any N > l.

Now we consider the adjacency matrix denoted by  $MG_l^{(r)}$  of the de Bruijn graph  $G_l^{(r)}$ [18]. The adjacency matrix  $MG_l^{(r)}$  of  $G_l^{(r)}$  is a  $r^l \times r^l$  matrix whose entries  $m_{ij}$  are given by

$$m_{ij} = \begin{cases} 1 & \text{if } v_i v_j \text{ is a directed edge} \\ 0 & \text{otherwise} \end{cases}$$

where  $v_i$  and  $v_j$  are vertices of  $G_l^{(r)}$  and  $v_i v_j$  denotes a directed edge which connects  $v_i$  and  $v_j$  in the direction from  $v_i$  to  $v_j$ . For example, the adjacency matrix  $MG_2^{(2)}$  of  $G_2^{(2)}$  is

$$MG_2^{(2)} = \begin{pmatrix} 1 & 1 & 0 & 0\\ 0 & 0 & 1 & 1\\ 1 & 1 & 0 & 0\\ 0 & 0 & 1 & 1 \end{pmatrix}$$
(2)

where we put  $v_1 := 00$ ,  $v_2 := 01$ ,  $v_3 := 10$  and  $v_4 := 11$ .

Next we introduce the weighted adjacency matrix denoted by  $M_R G_l^{(r)}$  of the de Bruijn graph  $G_l^{(r)}$  with the mapping  $\phi_R$  associated with the rule *R* of the cellular automaton  $\mathcal{A}_{l+1}^{(r)}$ . The entries  $m_{ii}$  of  $M_R G_l^{(r)}$  are given by

$$m_{ij} = \begin{cases} a_0 & \text{if } v_i v_j \text{ is a directed edge and } \phi_R(v_i v_j) = 0\\ a_1 & \text{if } v_i v_j \text{ is a directed edge and } \phi_R(v_i v_j) = 1\\ \vdots & \\ a_{r-1} & \text{if } v_i v_j \text{ is a directed edge and } \phi_R(v_i v_j) = r - 1\\ 0 & \text{otherwise.} \end{cases}$$

For example, the weighted adjacency  $M_{154}G_2^{(2)}$  of  $G_2^{(2)}$  with the mapping  $\phi_{154}$ , which is equivalent to the local transition function (1), is

$$M_{154}G_2^{(2)} = \begin{pmatrix} a_0 & a_1 & 0 & 0\\ 0 & 0 & a_0 & a_1\\ a_1 & a_0 & 0 & 0\\ 0 & 0 & a_0 & a_1 \end{pmatrix}.$$
(3)

Consider the tensor algebra  $T(W) = \bigoplus_{i=0}^{\infty} W^{\otimes i}$ , where *W* is the  $\mathbb{Z}$ -module generated by the weights  $a_0, a_1, \ldots, a_{r-1}$ . We regard the weighted adjacency matrix as a matrix over T(W) and define a product  $\otimes : M(T(W), n) \times M(T(W), n) \to M(T(W), n)$  of two  $n \times n$ matrices  $A = (\alpha_{ij})_{i,j=1,2,...,n} B = (\beta_{ij})_{i,j=1,2,...,n}$  over T(W) as

$$A \otimes B := \left(\sum_{k=1}^{n} \alpha_{ik} \otimes \beta_{kj}\right)_{i,j=1,2,\dots,n}$$

Then, for the  $L(\geq l)$ th power of the matrix  $M_R G_l^{(r)}$ ,

$$M_R G_l^{(r)\otimes L} := \underbrace{M_R G_l^{(r)} \otimes M_R G_l^{(r)} \otimes \cdots \otimes M_R G_l^{(r)}}_{L}$$

its entry in position (i, j),

$$\left(M_{R}G_{l}^{(r)\otimes L}\right)_{ij} = \sum_{k_{1},k_{2},\dots,k_{L-1}=1}^{r^{l}} \underbrace{m_{ik_{1}}\otimes m_{k_{1}k_{2}}\otimes\dots\otimes m_{k_{L-1}j}}_{L}$$
(4)

where  $m_{ik_1}, m_{k_1k_2}, \ldots, m_{k_{L-1}j} \in \{0, a_0, a_1, \ldots, a_{r-1}\}$ , is a non-commutative polynomial of degree L in  $a_0, a_1, \ldots, a_{r-1}$  with  $r^{L-1}$  terms of coefficient 1. Because, from the unique path property of the de Bruijn graph, all the entries of  $M_R G_l^{(r)\otimes l}$  are monomials of length l in  $a_0, a_1, \ldots, a_{r-1}$ , then, by multiplying  $M_R G_l^{(r)}$ , all the entries of  $M_R G_l^{(r)\otimes l+1}$  are polynomials of degree l+1 in  $a_0, a_1, \ldots, a_{r-1}$  with r terms of coefficient 1. Hence inductively we have the above fact. By definition of the weighted adjacency matrix and the product  $\otimes$ , it is clear that each term of the polynomial (4) corresponds to a walk of length L in the de Bruijn graph  $G_l^{(r)}$ . In particular, all the terms of the trace of  $M_R G_l^{(r)\otimes L}$  correspond one-to-one to all the closed walks of length L in  $G_l^{(r)}$ . Therefore, we obtain the following theorem:

**Theorem 1.** A rule of the cellular automaton  $\mathcal{A}_{l+1}^{(r)} = \langle N, \mathbb{Z}_r, E, \delta \rangle$  of cell size N is reversible if and only if all the  $r^N$  terms of  $\operatorname{Tr}\left[M_R G_l^{(r)\otimes N}\right]$ , which are monomials of degree N in  $a_0$ ,  $a_1, \ldots, a_{r-1}$ , are distinct.

In the next section, we show a necessary and sufficient condition for reversibility of ECA using theorem 1.

# 3. Reversibility of elementary cellular automaton

In this section, we concentrate on ECA. Each ECA rule is referred to the rule number R given by

$$R := \sum_{s_1=0}^{1} \sum_{s_2=0}^{1} \sum_{s_3=0}^{1} \delta_{\text{ECA}}(s_1, s_2, s_3) 2^{4s_1 + 2s_2 + s_3}$$

where  $\delta_{\text{ECA}} : \mathbb{Z}_2^3 \to \mathbb{Z}_2$  is the local transition function [10]. An ECA rule given by the local transition function (1) is referred to the number R = 154.

A mapping  $\phi_R : \mathcal{E} \to \mathbb{Z}_2$ , where  $\mathcal{E} := \{000, 001, 010, 011, 100, 101, 110, 111\}$  is the edge set of the de Bruijn graph  $G_2^{(2)}$ , is equivalent to the local transition function of an ECA rule. For example, the following mapping is equivalent to the rule 154:

$$\phi_{154}(\varepsilon_1) = 1 \qquad \phi_{154}(\varepsilon_2) = 0 \qquad \phi_{154}(\varepsilon_3) = 1 \qquad \phi_{154}(\varepsilon_4) = 0 \phi_{154}(\varepsilon_5) = 0 \qquad \phi_{154}(\varepsilon_6) = 1 \qquad \phi_{154}(\varepsilon_7) = 1 \qquad \phi_{154}(\varepsilon_8) = 0$$

where we put  $\varepsilon_1 := 111$ ,  $\varepsilon_2 := 110$ ,  $\varepsilon_3 := 011$ ,  $\varepsilon_4 := 101$ ,  $\varepsilon_5 := 010$ ,  $\varepsilon_6 := 100$ ,  $\varepsilon_7 := 001$ and  $\varepsilon_8 := 000$ .

From theorem 1, in order to show reversibility of an ECA rule for the cell size N, we have only to show that all the  $2^N$  terms of Tr  $[M_R G_2^{(2)\otimes N}]$ , which are monomials of degree N in  $a_0$  and  $a_1$ , are distinct. We see that if  $\phi_R(\varepsilon_1) = \phi_R(\varepsilon_8)$  for the loops  $\varepsilon_1$  and  $\varepsilon_8$ , then the configuration  $\phi_R^{\otimes N}(\varepsilon_1\varepsilon_1\cdots\varepsilon_1)$  coincides with  $\phi_R^{\otimes N}(\varepsilon_8\varepsilon_8\cdots\varepsilon_8)$  for any N. Therefore, such rules are never reversible for any N. There exist 128 such rules, which are referred to even numbers less than 128 or odd numbers greater than 128. Hence, in the following, we consider the rules referred to even numbers equally greater than 128 or odd numbers smaller than 128.

For the number of  $\varepsilon_i$  such that  $\phi_R(\varepsilon_i) = 1$ , we have the following lemma. The property of this lemma is equivalent to the notion of 'balancedness' of the local transition function, which is known for a necessary condition for reversibility [19].

**Lemma 1.** If the number of  $\varepsilon_i$  such that  $\phi_R(\varepsilon_i) = 1$  is not equal to 4 then the corresponding ECA rule is not reversible for infinitely many cell sizes.

**Proof.** We can assume  $\phi_R(\varepsilon_1) = 1$  and  $\phi_R(\varepsilon_8) = 0$ . Then there exist three cases satisfying the condition of lemma: the number of edges  $\varepsilon_i$  such that  $\phi_R(\varepsilon_i) = 1$  except for  $\varepsilon_1$  is 0, 1 or 2. The cases when the number of such  $\varepsilon_i$  is greater than 5 are reduced to the above cases by exchanging 0 and 1. If there is no edge  $\varepsilon_i$  such that  $\phi_R(\varepsilon_i) = 1$  then the corresponding rule is obviously non-reversible because we obtain two distinct closed walks of arbitrary length mapped into the same configuration by  $\phi_R$ .

Assume that there exists an edge  $\varepsilon_i$  (i = 2, 3, ..., 7) such that  $\phi_R(\varepsilon_i) = 1$ . If  $\phi_R(\varepsilon_5) = \phi_R(\varepsilon_6) = \phi_R(\varepsilon_7) = 0$  then the rule is not reversible for  $N \ge 3$ , because we obtain two distinct closed walks of length n + 3 mapped into the same configuration by  $\phi_R$ :

$$\phi_R^{\otimes n+3}(\varepsilon_7\varepsilon_5\varepsilon_6\underbrace{\varepsilon_8\cdots\varepsilon_8}_{n}) = \phi_R^{\otimes n+3}\underbrace{(\varepsilon_8\cdots\varepsilon_8)}_{n+3} = \underbrace{0\cdots0}_{n+3}.$$
(5)

Therefore if  $\phi_R(\varepsilon_2) = 1$ ,  $\phi_R(\varepsilon_3) = 1$  or  $\phi_R(\varepsilon_4) = 1$  then the rule is not reversible. Similarly, if  $\phi_R(\varepsilon_5) = 1$ ,  $\phi_R(\varepsilon_6) = 1$  or  $\phi_R(\varepsilon_7) = 1$  then the rule is not reversible.

Assume that there exist two edges  $\varepsilon_i$  (i = 2, 3, ..., 7) such that  $\phi_R(\varepsilon_i) = 1$ . Then there exist 15 cases. If the two edges which satisfy  $\phi_R(\varepsilon_i) = 1$  are chosen from  $\varepsilon_2$ ,  $\varepsilon_3$  and  $\varepsilon_4$  then the rule is not reversible because we obtain two distinct closed walks mapped into the same

configuration (5) by  $\phi_R$ . If we put  $\phi_R(\varepsilon_2) = \phi_R(\varepsilon_5) = 1$  or  $\phi_R(\varepsilon_3) = \phi_R(\varepsilon_5) = 1$  then we have

$$\phi_R^{\otimes n+3}(\varepsilon_7\varepsilon_5\varepsilon_6\underbrace{\varepsilon_8\cdots\varepsilon_8}_n)=\phi_R^{\otimes n+3}(\varepsilon_3\varepsilon_2\varepsilon_6\underbrace{\varepsilon_8\cdots\varepsilon_8}_{n-1}\varepsilon_7)=\underbrace{010\cdots0}_{n+3}$$

or

$$\phi_R^{\otimes n+3}(\varepsilon_7\varepsilon_5\varepsilon_6\underbrace{\varepsilon_8\cdots\varepsilon_8}_n)=\phi_R^{\otimes n+3}(\varepsilon_7\varepsilon_3\varepsilon_2\varepsilon_6\underbrace{\varepsilon_8\cdots\varepsilon_8}_{n-1})=\underbrace{010\cdots0}_{n+3}$$

therefore the rule is not reversible. In the remaining 10 cases, we similarly obtain two distinct closed walks of length  $N \ge 4$  mapped into the same configuration by  $\phi_R$  respectively. Hence the corresponding rules are not reversible.

Next we consider automorphisms on ECA. Automorphisms on ECA preserve reversibility of an ECA rule, that is, a reversible rule is mapped into another reversible rule by the automorphisms respectively. The graph automorphism  $\varrho_1 : \mathcal{E} \to \mathcal{E}$ ,

$$\varrho_1(\varepsilon_i) = \varepsilon_{9-i} \qquad i = 1, 2, \dots, 8$$

of the de Bruijn graph  $G_2^{(2)}$  introduced in section 2 (this automorphism is realized as the rotation of  $\pi$  in figure 1) induces an action on  $\phi_R : \mathcal{E} \to \mathbb{Z}_2$ , which is also denoted by  $\varrho_1$ :

$$\varrho_1(\phi_R(\varepsilon_i)) := \phi_R(\varrho_1(\varepsilon_i)) = \phi_R(\varepsilon_{9-i}) \qquad i = 1, 2, \dots, 8.$$
(6)

The mapping  $\rho_1$  acts on { $\phi_R | R = 0, 1, ..., 255$ } as a permutation, hence it can be regarded as an automorphism on ECA. The automorphism  $\rho_1$  maps each rule referred to an even number equally greater than 128, which satisfies  $\phi_R(\varepsilon_1) = 1$  and  $\phi_R(\varepsilon_8) = 0$ , into a rule referred to an odd number smaller than 128, which satisfies  $\phi_R(\varepsilon_1) = 0$  and  $\phi_R(\varepsilon_8) = 1$ . Therefore we only have to consider even rules equally greater than 128. In addition, we consider the reflection  $\sigma$ and the conjugation  $\tau_1$  introduced in section 2 [10]. The reflection  $\sigma$  is

$$\sigma : \delta(c(i-1), c(i), c(i+1)) \mapsto \delta(c(i+1), c(i), c(i-1)) \qquad i = 1, 2, \dots, N$$

and the conjugation  $\tau_1$ , which exchange 0 and 1, is

1

$$\tau_1 : \delta(c(i-1), c(i), c(i+1)) \mapsto 1 - \delta(1 - c(i-1), 1 - c(i), 1 - c(i+1))$$
  
$$i = 1, 2, \dots, N.$$

For example, the rule 154 is mapped into the rules 210, 166 and 89 by  $\sigma$ ,  $\tau_1$  and  $\rho_1$ , respectively.

Considering the above facts, we conclude that there exist 10 rules which may be reversible up to automorphisms. Since the rules 170 (right-shift) and 204 (identity) are obviously reversible and reversibility of the rule 150 has already been proved [14], we only have to consider the following seven rules:

$$42, 154, 156, 172, 178, 184, 232.$$
(7)

In the following, we show that only the rule 154 is reversible among the above list. At first, we show reversibility of the rule 154.

#### **Proposition 1.** The rule 154 ECA is reversible for the cell size $N \equiv 1 \pmod{2}$ .

**Proof.** We put N = 2k + 1 ( $k \in \mathbb{N}$ ). From theorem 1, in order to show reversibility of rule 154, we show that all the  $2^N$  terms of

$$\operatorname{Tr}\left[M_{154}G_{2}^{(2)\otimes N}\right] = \operatorname{Tr}\left[\begin{pmatrix}a_{0} & a_{1} & 0 & 0\\ 0 & 0 & a_{0} & a_{1}\\ a_{1} & a_{0} & 0 & 0\\ 0 & 0 & a_{0} & a_{1}\end{pmatrix}^{\otimes N}\right]$$
(8)

are distinct.

For k = 1, this is true as follows:

$$\operatorname{Tr}\left[M_{154}G_{2}^{(2)\otimes3}\right] = \operatorname{Tr}\begin{pmatrix}a_{0}a_{0}a_{0} + a_{1}a_{0}a_{1} & a_{0}a_{0}a_{1} + a_{1}a_{0}a_{0} & a_{0}a_{1}a_{0} + a_{1}a_{1}a_{0} & a_{0}a_{1}a_{1} + a_{1}a_{1}a_{1}\\a_{0}a_{1}a_{0} + a_{1}a_{0}a_{1} & a_{0}a_{1}a_{1} + a_{1}a_{0}a_{0} & a_{0}a_{0}a_{0} + a_{1}a_{1}a_{0} & a_{0}a_{0}a_{1} + a_{1}a_{1}a_{1}\\a_{0}a_{0}a_{1} + a_{1}a_{0}a_{0} & a_{0}a_{0}a_{0} + a_{1}a_{0}a_{1} & a_{0}a_{1}a_{0} + a_{1}a_{1}a_{0} & a_{0}a_{0}a_{1} + a_{1}a_{1}a_{1}\\a_{0}a_{1}a_{0} + a_{1}a_{0}a_{1} & a_{0}a_{1}a_{1} + a_{1}a_{0}a_{0} & a_{0}a_{0}a_{0} + a_{1}a_{1}a_{0} & a_{0}a_{0}a_{1} + a_{1}a_{1}a_{1}\\a_{0}a_{1}a_{0} + a_{1}a_{0}a_{1} & a_{0}a_{1}a_{1} + a_{1}a_{0}a_{0} & a_{0}a_{0}a_{0} + a_{1}a_{1}a_{0} & a_{0}a_{0}a_{1} + a_{1}a_{1}a_{1}\\a_{0}a_{1}a_{0} + a_{1}a_{0}a_{1} & a_{0}a_{1}a_{1} + a_{1}a_{0}a_{0} & a_{0}a_{0}a_{0} + a_{1}a_{1}a_{0} & a_{0}a_{0}a_{1} + a_{1}a_{1}a_{1}\\a_{0}a_{1}a_{0} + a_{1}a_{0}a_{1} & a_{0}a_{1}a_{1} + a_{1}a_{0}a_{0} & a_{0}a_{0}a_{0} + a_{1}a_{1}a_{0} & a_{0}a_{0}a_{1} + a_{1}a_{1}a_{1}\\a_{0}a_{1}a_{0} + a_{1}a_{0}a_{1} & a_{0}a_{1}a_{1} + a_{1}a_{0}a_{0} & a_{0}a_{0}a_{0} + a_{1}a_{1}a_{0} & a_{0}a_{0}a_{1} + a_{1}a_{1}a_{1}\\a_{0}a_{1}a_{0} + a_{1}a_{0}a_{1} & a_{0}a_{1}a_{1} + a_{1}a_{0}a_{0} & a_{0}a_{0}a_{0} + a_{1}a_{1}a_{0} & a_{0}a_{0}a_{1} + a_{1}a_{1}a_{1}\\a_{0}a_{0}a_{0} + a_{1}a_{0}a_{0} & a_{0}a_{0}a_{0} + a_{0}a_{0}a_{0} & a_{0}a_{$$

 $= a_0a_0a_0 + a_1a_0a_1 + a_0a_1a_1 + a_1a_0a_0 + a_0a_1a_0 + a_1a_1a_0 + a_0a_0a_1 + a_1a_1a_1$ 

(9)

We have the following lemma:

**Lemma 2.** Suppose N = 2k + 1 ( $k \in \mathbb{N}$ ). For  $M_{154}G_2^{(2)\otimes N}$ , we have

$$\begin{aligned} 1. \quad \sum_{j=1}^{4} \left( M_{154} G_2^{(2)\otimes N} \right)_{1j} &= \sum_{j=1}^{4} \left( M_{154} G_2^{(2)\otimes N} \right)_{2j} \\ &= \sum_{j=1}^{4} \left( M_{154} G_2^{(2)\otimes N} \right)_{3j} = \sum_{j=1}^{4} \left( M_{154} G_2^{(2)\otimes N} \right)_{4j} \\ 2. \quad \left( M_{154} G_2^{(2)\otimes N} \right)_{12} + \left( M_{154} G_2^{(2)\otimes N} \right)_{14} &= \left( M_{154} G_2^{(2)\otimes N} \right)_{22} + \left( M_{154} G_2^{(2)\otimes N} \right)_{24} \\ 3. \quad \left( M_{154} G_2^{(2)\otimes N} \right)_{13} &= \left( M_{154} G_2^{(2)\otimes N} \right)_{33} \\ 4. \quad \left( M_{154} G_2^{(2)\otimes N} \right)_{24} &= \left( M_{154} G_2^{(2)\otimes N} \right)_{44} \\ & \text{where } A_{ij} \text{ stands for the } (i, j) \text{-entry of } A. \end{aligned}$$

**Proof of lemma.** There exist  $2^N$  walks of length N in  $G_2^{(2)}$  whose first vertex is  $v_i$ , i = 1, 2, 3, 4. These walks are mapped into distinct elements of  $\mathbb{Z}_2^{\otimes N}$  by  $\phi_{154}$  because two edges starting from any vertex are mapped into distinct elements of  $\mathbb{Z}_2$  by  $\phi_{154}$ . Moreover, all the  $2^N$  walks of length N whose first vertex is  $v_i$  correspond one-to-one to all the  $2^N$  terms of the sum of the *i*th row of  $M_{154}G_2^{(2)\otimes N}$ :

$$\sum_{j=1}^{4} \left( M_{154} G_2^{(2)\otimes N} \right)_{ij} \qquad i = 1, 2, 3, 4.$$
(10)

Therefore all the  $2^N$  terms of (10), which are monomials of degree N in  $a_0$  and  $a_1$ , are distinct for any i = 1, 2, 3, 4. On the other hand, there exist  $2^N$  monomials of degree N in  $a_0$  and  $a_1$ , and these monomials constitute the terms of (10). Hence (10) is the same for all i = 1, 2, 3, 4. Therefore the statement 1 is true.

From (9), the statements 2, 3 and 4 are true for k = 1. Assume that these are true for k. For simplicity, we put  $A := M_{154}G_2^{(2)\otimes N}$  and  $C := \sum_{j=1}^4 (M_{154}G_2^{(2)\otimes N})_{1j}$ . Using

$$M_{154}G_2^{(2)\otimes 2} = \begin{pmatrix} a_0a_0 & a_0a_1 & a_1a_0 & a_1a_1 \\ a_0a_1 & a_0a_0 & a_1a_0 & a_1a_1 \\ a_1a_0 & a_1a_1 & a_0a_0 & a_0a_1 \\ a_0a_1 & a_0a_0 & a_1a_0 & a_1a_1 \end{pmatrix}$$

and the assumption of induction, we have

$$(M_{154}G_2^{(2)\otimes N+2})_{13} = (A \otimes M_{154}G_2^{(2)\otimes 2})_{13} = \{A_{11} + A_{12} + A_{14}\}a_1a_0 + A_{13}a_0a_0 = \{C - A_{13}\}a_1a_0 + A_{13}a_0a_0 = \{C - A_{33}\}a_1a_0 + A_{33}a_0a_0$$

$$= \{A_{31} + A_{32} + A_{34}\}a_1a_0 + A_{33}a_0a_0$$
  
=  $(A \otimes M_{154}G_2^{(2)\otimes 2})_{33}$   
=  $(M_{154}G_2^{(2)\otimes N+2})_{33}$ .

Similarly, we obtain  $(M_{154}G_2^{(2)\otimes N+2})_{24} = (M_{154}G_2^{(2)\otimes N+2})_{44}$ . Moreover, we have

$$\begin{split} \left( M_{154} G_2^{(2) \otimes N+2} \right)_{12} + \left( M_{154} G_2^{(2) \otimes N+2} \right)_{14} \\ &= \left( A \otimes M_{154} G_2^{(2) \otimes 2} \right)_{12} + \left( A \otimes M_{154} G_2^{(2) \otimes 2} \right)_{14} \\ &= \left\{ A_{11} + A_{13} \right\} (a_0 a_1 + a_1 a_1) + \left\{ A_{12} + A_{14} \right\} (a_0 a_0 + a_1 a_1) \\ &= \left\{ C - (A_{12} + A_{14}) \right\} (a_0 a_1 + a_1 a_1) + \left\{ A_{12} + A_{14} \right\} (a_0 a_0 + a_1 a_1) \\ &= \left\{ C - (A_{22} + A_{24}) \right\} (a_0 a_1 + a_1 a_1) + \left\{ A_{22} + A_{24} \right\} (a_0 a_0 + a_1 a_1) \\ &= \left\{ A \otimes M_{154} G_2^{(2) \otimes 2} \right\}_{22} + \left( A \otimes M_{154} G_2^{(2) \otimes 2} \right)_{24} \\ &= \left( M_{154} G_2^{(2) \otimes N+2} \right)_{22} + \left( M_{154} G_2^{(2) \otimes N+2} \right)_{24}. \end{split}$$

Thus the lemma is proved.

From the above lemma, we have

$$\operatorname{Tr}\left[M_{154}G_{2}^{(2)\otimes N}\right] = \left(M_{154}G_{2}^{(2)\otimes N}\right)_{11} + \left(M_{154}G_{2}^{(2)\otimes N}\right)_{22} + \left(M_{154}G_{2}^{(2)\otimes N}\right)_{33} + \left(M_{154}G_{2}^{(2)\otimes N}\right)_{44} \\ = \left(M_{154}G_{2}^{(2)\otimes N}\right)_{11} + \left(M_{154}G_{2}^{(2)\otimes N}\right)_{22} + \left(M_{154}G_{2}^{(2)\otimes N}\right)_{13} + \left(M_{154}G_{2}^{(2)\otimes N}\right)_{24} \\ = \left(M_{154}G_{2}^{(2)\otimes N}\right)_{11} + \left(M_{154}G_{2}^{(2)\otimes N}\right)_{12} + \left(M_{154}G_{2}^{(2)\otimes N}\right)_{13} + \left(M_{154}G_{2}^{(2)\otimes N}\right)_{14}.$$

As in the proof of the statement 1 of the above lemma, all the  $2^N$  terms of the last formula are distinct. Thus, for any  $N \equiv 1 \pmod{2}$ , all the  $2^N$  terms of  $\text{Tr}\left[M_{154}G_2^{(2)\otimes N}\right]$  are distinct. Hence the rule 154 ECA is reversible for the cell size  $N \equiv 1 \pmod{2}$ .

Next we show that the rules 142, 156, 172, 178, 184 and 232 are not reversible for any cell size  $N \ge 4$ . For the rule 142, the mapping  $\phi_{142}$  is as follows:

$$\phi_{142}(\varepsilon_1) = \phi_{142}(\varepsilon_3) = \phi_{142}(\varepsilon_5) = \phi_{142}(\varepsilon_7) = 1$$
  
$$\phi_{142}(\varepsilon_2) = \phi_{142}(\varepsilon_4) = \phi_{142}(\varepsilon_6) = \phi_{142}(\varepsilon_8) = 0.$$

Two closed walks of length 4,  $\varepsilon_2 \varepsilon_4 \varepsilon_3 \varepsilon_1$  and  $\varepsilon_2 \varepsilon_6 \varepsilon_7 \varepsilon_3$ , are mapped into the same configuration 0011 by  $\phi_{142}$ , hence the rule 142 is not reversible for N = 4. Moreover, from the above closed walks of length 4, we can obtain two closed walks of length N > 4 mapped into the same configuration by  $\phi_{142}$ :

$$\phi_{142}^{\otimes N}(\varepsilon_2\varepsilon_4\varepsilon_3\varepsilon_1\underbrace{\varepsilon_1\cdots\varepsilon_1}_{N-4}) = \phi_{142}^{\otimes N}(\varepsilon_2\varepsilon_6\varepsilon_7\varepsilon_3\underbrace{\varepsilon_1\cdots\varepsilon_1}_{N-4}) = 0011\underbrace{1\cdots1}_{N-4}.$$

Therefore the rule 142 is not reversible for any  $N \ge 4$ . For the rule 156, the mapping  $\phi_{156}$  is as follows:

$$\phi_{156}(\varepsilon_1) = \phi_{156}(\varepsilon_3) = \phi_{156}(\varepsilon_5) = \phi_{156}(\varepsilon_6) = 1$$
  
$$\phi_{156}(\varepsilon_2) = \phi_{156}(\varepsilon_4) = \phi_{156}(\varepsilon_7) = \phi_{156}(\varepsilon_8) = 0.$$

**Table 1.** All the reversible ECA rules with periodic boundary conditions and the cell sizes for which the rules are reversible. The rules below the automorphisms  $\sigma$ ,  $\tau_1$ ,  $\rho_1$  and their compositions are mapped into the left-most rules by them respectively.

SILC
1, 2 (mod 3)
1 (mod 2)
$V \in \mathbb{N}$
$V \in \mathbb{N}$

We can obtain two distinct closed walks mapped into the same configuration of lengths 4, 5, 6 and 7 by  $\phi_{156}$  respectively:

$$\phi_{156}^{\otimes 4}(\varepsilon_2\varepsilon_6\varepsilon_7\varepsilon_3) = \phi_{156}^{\otimes 4}(\varepsilon_4\varepsilon_5\varepsilon_4\varepsilon_5) = 0101$$
  

$$\phi_{156}^{\otimes 5}(\varepsilon_2\varepsilon_6\varepsilon_8\varepsilon_7\varepsilon_3) = \phi_{156}^{\otimes 5}(\varepsilon_4\varepsilon_3\varepsilon_2\varepsilon_4\varepsilon_5) = 01001$$
  

$$\phi_{156}^{\otimes 6}(\varepsilon_2\varepsilon_6\varepsilon_7\varepsilon_5\varepsilon_4\varepsilon_3) = \phi_{156}^{\otimes 6}(\varepsilon_4\varepsilon_5\varepsilon_4\varepsilon_5\varepsilon_4\varepsilon_5) = 010101$$
  

$$\phi_{156}^{\otimes 7}(\varepsilon_2\varepsilon_6\varepsilon_7\varepsilon_3\varepsilon_2\varepsilon_4\varepsilon_3) = \phi_{156}^{\otimes 7}(\varepsilon_4\varepsilon_5\varepsilon_4\varepsilon_3\varepsilon_2\varepsilon_4\varepsilon_5) = 0101001.$$

Consider two walks  $\varepsilon_6 \varepsilon_7 \varepsilon_3 \varepsilon_2 \cdots \varepsilon_6 \varepsilon_7 \varepsilon_3 \varepsilon_2$  and  $\varepsilon_5 \varepsilon_4 \varepsilon_5 \varepsilon_4 \cdots \varepsilon_5 \varepsilon_4 \varepsilon_5 \varepsilon_4$  of length  $4k \ (k \in \mathbb{N})$ . Note that these two walks mapped into the same configuration by  $\phi_{156}$ :

$$\phi_{156}^{\otimes 4k}(\varepsilon_6\varepsilon_7\varepsilon_3\varepsilon_2\cdots\varepsilon_6\varepsilon_7\varepsilon_3\varepsilon_2) = \phi_{156}^{\otimes 4k}(\varepsilon_5\varepsilon_4\varepsilon_5\varepsilon_4\cdots\varepsilon_5\varepsilon_4\varepsilon_5\varepsilon_4) = 1010\cdots1010.$$

Inserting  $\varepsilon_6\varepsilon_7\varepsilon_3\varepsilon_2\cdots\varepsilon_6\varepsilon_7\varepsilon_3\varepsilon_2$  and  $\varepsilon_5\varepsilon_4\varepsilon_5\varepsilon_4\cdots\varepsilon_5\varepsilon_4\varepsilon_5\varepsilon_4$  between the first and the second edges of  $\varepsilon_2\varepsilon_6\varepsilon_7\varepsilon_3$  and  $\varepsilon_4\varepsilon_5\varepsilon_4\varepsilon_5$  respectively, we obtain two distinct closed walks of length 4k + 4 mapped into the same configuration by  $\phi_{156}$ . Similarly, from the above closed walks of lengths 5, 6 and 7, we obtain distinct closed walks of lengths 4k + 5, 4k + 6 and 4k + 7 mapped into the same configurations by  $\phi_{156}$ , respectively. Hence the rule 156 is not reversible for any  $N \ge 4$ .

We can similarly show non-reversibility for  $N \ge 4$  of the rules 172, 178, 184 and 232. Thus we conclude that only the rule 154 is reversible among the seven rules in (7).

Now we will obtain all reversible ECA rules from the reversible rules 150, 154, 170 and 204 using the automorphisms on ECA. The rules 210, 166 and 180 are mapped into the rule 154 by the reflection  $\sigma$ , the conjugation  $\tau_1$  and their composition, respectively. Similarly, the rule 240 is mapped into the rule 170 by  $\sigma$ , and the rule 240 is invariant with respect to  $\tau_1$ . The rules 150 and 204 are invariant with respect to both  $\sigma$  and  $\tau_1$ . In addition, we consider the automorphism  $\rho_1$  (6) induced by the graph automorphism  $\rho_1$  of the de Bruijn graph  $G_2^{(2)}$ . Each reversible even rule equally greater than 128 is mapped into a reversible odd rule smaller than 128 by  $\rho_1$ . Thus we obtain the following theorem.

# **Theorem 2.** There exist exactly 16 reversible ECA rules for infinitely many cell sizes (see table 1).

The rules 204 and 170 are trivial, and the rule 150 is additive, that is, whose local transition function can be regarded as a linear function on  $\mathbb{Z}_2$ . Hence only the rule 154 is considered to be essentially nonlinear. Therefore, it is expected that the rule 154 has interesting properties. We will discuss solutions, periods of solutions and conserved quantities of the rule 154 in a forthcoming paper.

# 4. A sufficient condition for reversibility of the cellular automaton $\mathcal{A}_2^{(3)}$

In this section, we show a sufficient condition for reversibility of the cellular automaton  $\mathcal{A}_2^{(3)} = \langle N, \mathbb{Z}_3, \{0, 1\}, \delta_2^{(3)} \rangle$  with periodic boundary conditions. The sufficient condition



**Figure 3.** The de Bruijn graph  $G_1^{(3)}$ 

is a straightforward extension of a sufficient condition for reversibility of ECA  $\left(\mathcal{A}_3^{(2)}\right)$  to  $\mathcal{A}_2^{(3)}$ . Observing the weighted adjacency matrices  $M_R G_2^{(2)}$  of the de Bruijn graph  $G_2^{(2)}$  with the mapping  $\phi_R$  associated with the reversible rules, we obtain the following proposition concerning a sufficient condition for reversibility of ECA.

**Proposition 2.** If the weighted adjacency matrix  $M_R G_2^{(2)}$  of the de Bruijn graph  $G_2^{(2)}$  with the mapping  $\phi_R$  associated with an ECA rule R satisfies

$$\sum_{i=1}^{n} \left( M_R G_2^{(2)} \right)_{ij} = \operatorname{Tr} \left[ M_R G_2^{(2)} \right] = a_0 + a_1 \qquad for \quad i = 1, 2, 3, 4$$

or

$$\sum_{i=1}^{4} \left( M_R G_2^{(2)} \right)_{ij} = \operatorname{Tr} \left[ M_R G_2^{(2)} \right] = a_0 + a_1 \qquad for \quad j = 1, 2, 3, 4$$

then the rule R is reversible for infinitely many cell sizes.

The reversible rules 150, 154 and 170 satisfy this proposition. Since the conditions of proposition 2 are invariant with respect to the three automorphisms (the reflection  $\sigma$ , the conjugation  $\tau$  and the graph automorphism  $\rho_l$ ), all their automorphic rules (see table 1) also satisfy this proposition. The only counterexample is the trivial rule 204. Actually, the weighted adjacency matrix  $M_{204}G_2^{(2)}$  does not satisfy the condition of proposition 2 as follows:

$$M_{204}G_2^{(2)} = \begin{pmatrix} a_0 & a_0 & 0 & 0\\ 0 & 0 & a_1 & a_1\\ a_0 & a_0 & 0 & 0\\ 0 & 0 & a_1 & a_1 \end{pmatrix}$$

Therefore, the condition is not necessary for reversibility. Now we consider the cellular automaton  $\mathcal{A}_2^{(3)} = \langle N, \mathbb{Z}_3, \{0, 1\}, \delta_2^{(3)} \rangle$ . The de Bruijn graph associated with  $\mathcal{A}_2^{(3)}$  is  $G_1^{(3)}$  (see figure 3). The adjacency matrix of  $G_1^{(3)}$  is

$$MG_1^{(3)} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

where we put  $v_1 := 0$ ,  $v_2 := 1$  and  $v_3 := 2$ . We also consider the weighted adjacency matrix  $M_R G_1^{(3)}$  of  $G_1^{(3)}$  with the mapping  $\phi_R$  associated with the rule *R* of  $\mathcal{A}_2^{(3)}$ . Each rule is referred to the number *R* given by

$$R := \sum_{s_1=0}^{2} \sum_{s_2=0}^{2} \delta_2^{(3)}(s_1, s_2) 3^{3s_1+s_2}$$

where  $\delta_2^{(3)}$  is the local transition function. For example, for the mapping  $\phi_{14001}$  associated with the rule 14001

$$\begin{aligned} \phi_{14001}(\varepsilon_1 := 22) &= 2 & \phi_{14001}(\varepsilon_2 := 21) = 0 & \phi_{14001}(\varepsilon_3 := 20) = 1 \\ \phi_{14001}(\varepsilon_4 := 12) &= 0 & \phi_{14001}(\varepsilon_5 := 11) = 1 & \phi_{14001}(\varepsilon_6 := 10) = 2 \\ \phi_{14001}(\varepsilon_7 := 02) &= 1 & \phi_{14001}(\varepsilon_8 := 01) = 2 & \phi_{14001}(\varepsilon_9 := 00) = 0 \end{aligned}$$

the weighted adjacency matrix  $M_{14001}G_1^{(3)}$  is

$$M_{14001}G_1^{(3)} = \begin{pmatrix} a_0 & a_2 & a_1 \\ a_2 & a_1 & a_0 \\ a_1 & a_0 & a_2 \end{pmatrix}.$$

We obtain the following proposition concerning a sufficient condition for reversibility of  $\mathcal{A}_2^{(3)}$  and is a straightforward extension of proposition 2 for ECA to  $\mathcal{A}_2^{(3)}$ .

**Proposition 3.** If the weighted adjacency matrix  $M_R G_1^{(3)}$  of the de Bruijn graph  $G_1^{(3)}$  with the mapping  $\phi_R$  associated with a rule R of the cellular automaton  $\mathcal{A}_2^{(3)}$  satisfies

$$\sum_{j=1}^{3} \left( M_R G_1^{(3)} \right)_{ij} = \operatorname{Tr} \left[ M_R G_1^{(3)} \right] = a_0 + a_1 + a_2 \qquad for \quad i = 1, 2, 3 \tag{11}$$

or

$$\sum_{i=1}^{3} \left( M_R G_1^{(3)} \right)_{ij} = \operatorname{Tr} \left[ M_R G_1^{(3)} \right] = a_0 + a_1 + a_2 \qquad for \quad j = 1, 2, 3$$
(12)

then the rule R is reversible for infinitely many cell sizes.

**Proof.** Assume that  $M_R G_1^{(3)}$  satisfies the condition (11). There exist three cases: (i) all the three rows of  $M_R G_1^{(3)}$  are the same; (ii) only two rows are the same and (iii) all the three rows are distinct. Remark that the condition (11) is equivalent to the condition that all the three edges starting from any vertex of  $G_1^{(3)}$  are mapped into distinct element of  $\mathbb{Z}_3$  by  $\phi_R$ . Hence if (11) holds then

$$\sum_{i=1}^{3} \left( M_R G_1^{(3)\otimes N} \right)_{1i} = \sum_{i=1}^{3} \left( M_R G_1^{(3)\otimes N} \right)_{2i} = \sum_{i=1}^{3} \left( M_R G_1^{(3)\otimes N} \right)_{3i}$$
(13)

for any N. Moreover, (11) ensures that all the  $3^N$  terms of each formula in (13), which are monomials of degree N in  $a_0$ ,  $a_1$  and  $a_2$ , are distinct (see proof of lemma 2). In the case (i),  $M_R G_1^{(3)}$  has the form:

$$M_R G_1^{(3)} = \begin{pmatrix} \alpha & \beta & \gamma \\ \alpha & \beta & \gamma \\ \alpha & \beta & \gamma \end{pmatrix} \quad \alpha, \beta, \gamma \in \{a_0, a_1, a_2\} \quad \alpha \neq \beta \neq \gamma.$$
(14)

Then, for any  $N \in \mathbb{N}$ , we have

$$\left(M_R G_1^{(3)\otimes N}\right)_{1j} = \left(M_R G_1^{(3)\otimes N}\right)_{2j} = \left(M_R G_1^{(3)\otimes N}\right)_{3j} \quad \text{for} \quad j = 1, 2, 3.$$
There is a static set of the s

Therefore we obtain

$$\operatorname{Tr}\left[M_{R}G_{1}^{(3)\otimes N}\right] = \sum_{j=1}^{5} \left(M_{R}G_{1}^{(3)\otimes N}\right)_{1j}$$
(16)

On reversibility of cellular automata with periodic boundary conditions

$$=\sum_{j=1}^{3} \left( M_R G_1^{(3)\otimes N} \right)_{2j} \tag{17}$$

$$=\sum_{j=1}^{3} \left( M_R G_1^{(3)\otimes N} \right)_{3j}.$$
 (18)

Since all the terms on the right-hand side of (16), (17) and (18) are distinct, respectively, the rule *R* whose weighted adjacency matrix  $M_R G_1^{(3)}$  has the form (14) is reversible for any  $N \in \mathbb{N}$ .

In the case (ii),  $M_R G_1^{(3)}$  has the following three forms:

(I) 
$$\begin{pmatrix} \alpha & \beta & \gamma \\ \alpha & \beta & \gamma \\ \beta & \alpha & \gamma \end{pmatrix}$$
 (II)  $\begin{pmatrix} \alpha & \beta & \gamma \\ \gamma & \beta & \alpha \\ \alpha & \beta & \gamma \end{pmatrix}$  (III)  $\begin{pmatrix} \alpha & \gamma & \beta \\ \alpha & \beta & \gamma \\ \alpha & \beta & \gamma \end{pmatrix}$  (19)

where,  $\alpha, \beta, \gamma \in \{a_0, a_1, a_2\}, \alpha \neq \beta \neq \gamma$ . Then  $M_R G_1^{(3) \otimes 2}$  are

$$(I) \begin{pmatrix} \alpha \alpha + \beta \alpha + \gamma \beta & \alpha \beta + \beta \beta + \gamma \alpha & (\alpha + \beta + \gamma)\gamma \\ \alpha \alpha + \beta \alpha + \gamma \beta & \alpha \beta + \beta \beta + \gamma \alpha & (\alpha + \beta + \gamma)\gamma \\ \alpha \alpha + \beta \alpha + \gamma \beta & \alpha \beta + \beta \beta + \gamma \alpha & (\alpha + \beta + \gamma)\gamma \end{pmatrix}$$

$$(II) \begin{pmatrix} \alpha \alpha + \beta \gamma + \gamma \alpha & (\alpha + \beta + \gamma)\beta & \alpha \gamma + \beta \alpha + \gamma \gamma \\ \alpha \alpha + \beta \gamma + \gamma \alpha & (\alpha + \beta + \gamma)\beta & \alpha \gamma + \beta \alpha + \gamma \gamma \\ \alpha \alpha + \beta \gamma + \gamma \alpha & (\alpha + \beta + \gamma)\beta & \alpha \gamma + \beta \alpha + \gamma \gamma \end{pmatrix}$$

$$(III) \begin{pmatrix} (\alpha + \beta + \gamma)\alpha & \alpha \gamma + \gamma \beta + \beta \beta & \alpha \beta + \gamma \gamma + \beta \gamma \\ (\alpha + \beta + \gamma)\alpha & \alpha \gamma + \gamma \beta + \beta \beta & \alpha \beta + \gamma \gamma + \beta \gamma \\ (\alpha + \beta + \gamma)\alpha & \alpha \gamma + \gamma \beta + \beta \beta & \alpha \beta + \gamma \gamma + \beta \gamma \end{pmatrix}$$

respectively. Therefore, for any  $N \in \mathbb{N}$ , we obtain (15). Thus (16), (17) and (18) hold, and reversibility of the corresponding rule *R* immediately follows. In the case (iii),  $M_R G_1^{(3)}$  is reduced to the following four forms:

(I) 
$$\begin{pmatrix} \alpha & \beta & \gamma \\ \gamma & \beta & \alpha \\ \beta & \alpha & \gamma \end{pmatrix}$$
 (II)  $\begin{pmatrix} \alpha & \gamma & \beta \\ \alpha & \beta & \gamma \\ \beta & \alpha & \gamma \end{pmatrix}$   
(III)  $\begin{pmatrix} \alpha & \gamma & \beta \\ \gamma & \beta & \alpha \\ \alpha & \beta & \gamma \end{pmatrix}$  (IV)  $\begin{pmatrix} \alpha & \gamma & \beta \\ \gamma & \beta & \alpha \\ \beta & \alpha & \gamma \end{pmatrix}$  (20)

where  $\alpha, \beta, \gamma \in \{a_0, a_1, a_2\} \alpha \neq \beta \neq \gamma$ . Let  $M_R G_1^{(3)}$  be the form (I). Then

$$(M_R G_1^{(3)})_{12} = (M_R G_1^{(3)})_{22} \qquad (M_R G_1^{(3)})_{13} = (M_R G_1^{(3)})_{33}$$

and

$$(M_R G_1^{(3)\otimes 2})_{12} = (M_R G_1^{(3)\otimes 2})_{32} \qquad (M_R G_1^{(3)\otimes 2})_{13} = (M_R G_1^{(3)\otimes 2})_{23}$$

hold. From these relations and (13), we have

$$\left(M_R G_1^{(3)\otimes 3}\right)_{12} = \left(M_R G_1^{(3)\otimes 3}\right)_{22} \tag{6}$$

$$(M_R G_1^{(3)\otimes 3})_{13} = (M_R G_1^{(3)\otimes 3})_{33}.$$

Hence, for any  $N \equiv 1 \pmod{2}$ , inductively we have

$$\left(M_R G_1^{(3)\otimes N}\right)_{12} = \left(M_R G_1^{(3)\otimes N}\right)_{22} \qquad \left(M_R G_1^{(3)\otimes N}\right)_{13} = \left(M_R G_1^{(3)\otimes N}\right)_{33}$$

**Table 2.** Reversible rules of the cellular automaton  $A_2^{(3)}$  with periodic boundary conditions and the cell sizes for which the rules are reversible. All their automorphic rules are reversible.

Rule	Cell size				
7995, 10179, 1088, 19071, 19305	All N				
7527, 8229, 8697, 14001, 14703	$N \equiv 1 \; (\text{mod } 2)$				

Therefore (16) holds. In the remaining cases (II), (III) and (IV), we also obtain (16). Therefore, the corresponding rule *R* is reversible for any  $N \equiv 1 \pmod{2}$ .

For the condition (12), reversibility of the corresponding rule is similarly shown.  $\Box$ 

If we assume  $\phi_R(\varepsilon_9 = 00) = 0$ ,  $\phi_R(\varepsilon_5 = 11) = 1$  and  $\phi_R(\varepsilon_1 = 22) = 2$ , then there exist  $2^3$  rules satisfying (11). Since there exist 3! permutations on  $\{\phi_R(00), \phi_R(11), \phi_R(22)\} = \{0, 1, 2\}$ , there exist  $2^3 \times 3! = 48$  rules satisfying (11). This is also true for (12). But there exist 3! rules which satisfy both (11) and (12). Therefore, there exist  $48 \times 2 - 3! = 90$  rules satisfying (11) or (12). From the graph automorphisms  $\varrho_i(i = 1, 2)$  of  $G_2^{(3)}$ ,

$$\varrho_i(\alpha_1 \alpha_2) = (\alpha_1 + i)(\alpha_2 + i) \pmod{3} \qquad i = 1, 2$$

where  $\alpha_1 \alpha_2$  is an edge of  $G_1^{(3)}$ , an automorphism on  $\mathcal{A}_2^{(3)}$  denoted also by  $\rho_i$  is induced:

$$\varrho_i(\phi(\alpha_1\alpha_2)) := \phi(\varrho_i(\alpha_1\alpha_2)) \qquad i = 1, 2.$$

Moreover, there exist another automorphism on  $\mathcal{A}_2^{(3)}$ , the reflection  $\sigma$  and the conjugation  $\tau_1$  and  $\tau_2$ , which are introduced in section 2. Considering these automorphisms, we conclude that there exist 10 rules which satisfy (11) or (12) up to automorphisms. These 10 rules are listed in table 2.

Since the reversibility condition for  $\mathcal{A}_{2}^{(3)}$  is obtained by straightforward extension of the reversibility condition for ECA to  $\mathcal{A}_{2}^{(3)}$ , it is expected that we can obtain sufficient conditions for reversibility of the cellular automata  $\mathcal{A}_{l+1}^{(r)} = \langle N, \mathbb{Z}_r, \{e_1, e_2, \ldots, e_{l+1}\}, \delta \rangle$  for greater r and l in the same manner. However, this is not so easy. Extending propositions 2 and 3 straightforwardly, we obtain the following condition which is expected to be a sufficient condition for reversibility of  $\mathcal{A}_{l+1}^{(r)}$ :

**Condition 1.** The weighted adjacency matrix  $M_R G_l^{(r)}$  of the de Bruijn graph  $G_l^{(r)}$  with the mapping  $\phi_R$  associated with a rule R of the cellular automaton  $\mathcal{A}_{l+1}^{(r)}$  satisfies

$$\sum_{j=1}^{r^{\prime}} \left( M_R G_l^{(r)} \right)_{ij} = \operatorname{Tr} \left[ M_R G_l^{(r)} \right] = \sum_{k=0}^{r-1} a_k \qquad for \quad i = 1, 2, \dots, r^{\prime}$$

or

$$\sum_{i=1}^{r^{l}} \left( M_{R} G_{l}^{(r)} \right)_{ij} = \operatorname{Tr} \left[ M_{R} G_{l}^{(r)} \right] = \sum_{k=0}^{r-1} a_{k} \qquad for \quad j = 1, 2, \dots, r^{l}.$$

But this condition is not sufficient. In the case of  $\mathcal{A}_4^{(2)} = \langle N, \mathbb{Z}_2, \{-1, 0, 1, 2\}, \delta_4^{(2)} \rangle$ , although there exist 35 rules up to automorphisms which satisfy the above condition, only 6 of them are reversible. The reversible rules are listed in table 3. Each rule is referred to the number *R* given by

$$R := \sum_{s_1=0}^{1} \sum_{s_2=0}^{1} \sum_{s_3=0}^{1} \sum_{s_4=0}^{1} \delta_4^{(2)}(s_1, s_2, s_3, s_4) 2^{2^3 s_1 + 2^2 s_2 + 2s_3 + s_4}$$

**Table 3.** Reversible rules of the cellular automaton  $\mathcal{A}_4^{(2)}$  with periodic boundary conditions and the cell sizes for which the rules are reversible. All their automorphic rules are reversible.

Cell size
All N
$N \equiv 1 \pmod{2}$
$N \equiv 1, 2 \pmod{3}$
$N \equiv 1, 2, 3, 4, 5, 6 \pmod{7}$

where  $\delta_4^{(2)}$  is the local transition function. The weighted adjacency matrices of the de Bruijn graph  $G_3^{(2)}$  associated with the reversible rules,  $M_{65280}G_3^{(2)}$ ,  $M_{53040}G_3^{(2)}$ ,  $M_{48960}G_3^{(2)}$ ,  $M_{49980}G_3^{(2)}$ ,  $M_{61200}G_3^{(2)}$  and  $M_{42330}G_3^{(2)}$  are as follows:

$(a_0)$	$a_0$	0	0	0	0	0	0 \	$(a_0)$	$a_0$	0	0	0	0	0	0 \
0	0	$a_0$	$a_0$	0	0	0	0	0	0	$a_0$	$a_0$	0	0	0	0
0	0	0	0	$a_0$	$a_0$	0	0	0	0	0	0	$a_1$	$a_1$	0	0
0	0	0	0	0	0	$a_0$	$a_0$	0	0	0	0	0	0	$a_0$	$a_0$
$a_1$	$a_1$	0	0	0	0	0	0	$a_1$	$a_1$	0	0	0	0	0	0
0	0	$a_1$	$a_1$	0	0	0	0	0	0	$a_1$	$a_1$	0	0	0	0
0	0	0	0	$a_1$	$a_1$	0	0	0	0	0	0	$a_0$	$a_0$	0	0
$\langle 0 \rangle$	0	0	0	0	0	$a_1$	$a_1$	$\langle 0 \rangle$	0	0	0	0	0	$a_1$	$a_1$
$(a_0)$	$a_0$	0	0	0	0	0	0)	$(a_0)$	$a_0$	0	0	0	0	0	0 \
0	0	$a_0$	$a_0$	0	0	0	0	0	0	$a_1$	$a_1$	0	0	0	0
0	0	0	0	$a_0$	$a_0$	0	0	0	0	0	0	$a_1$	$a_1$	0	0
0	0	0	0	0	0	$a_1$	$a_0$	0	0	0	0	0	0	$a_0$	$a_0$
$a_1$	$a_1$	0	0	0	0	0	0	$a_1$	$a_1$	0	0	0	0	0	0
0	0	$a_1$	$a_1$	0	0	0	0	0	0	$a_0$	$a_0$	0	0	0	0
0	0	0	0	$a_1$	$a_1$	0	0	0	0	0	0	$a_0$	$a_0$	0	0
0/	0	0	0	0	0	$a_0$	$a_1$	0	0	0	0	0	0	$a_1$	$a_1$
$(a_0)$	$a_0$	0	0	0	0	0	0)	$(a_0)$	$a_1$	0	0	0	0	0	0 \
0	0	$a_0$	$a_0$	0	0	0	0	0	0	$a_0$	$a_1$	0	0	0	0
0	0	0	0	$a_1$	$a_0$	0	0	0	0	0	0	$a_1$	$a_0$	0	0
0	0	0	0	0	0	$a_0$	$a_0$	0	0	0	0	0	0	$a_1$	$a_0$
$a_1$	$a_1$	0	0	0	0	0	0	$a_1$	$a_0$	0	0	0	0	0	0
0	0	$a_1$	$a_1$	0	0	0	0	0	0	$a_1$	$a_0$	0	0	0	0
0	0	0	0	$a_0$	$a_1$	0	0	0	0	0	0	$a_0$	$a_1$	0	0
0	0	0	0	0	0	$a_1$	$a_1$	$\langle 0 \rangle$	0	0	0	0	0	$a_0$	$a_1$

where we put  $v_1 := 111$ ,  $v_2 := 110$ ,  $v_3 := 101$ ,  $v_4 := 100$ ,  $v_5 := 011$ ,  $v_6 := 010$ ,  $v_7 := 001$ and  $v_8 := 000$ . For general *r* and *l*, it is expected that some of the rules which satisfy condition 1 are reversible.

### 5. Conclusion

We give a one-to-one correspondence between all the configurations of the cellular automaton  $\mathcal{A}_{l+1}^{(r)} = \langle N, \mathbb{Z}_r, \{e_1, e_2, \dots, e_{l+1}\}, \delta \rangle$  with periodic boundary conditions and all the  $r^N$  terms

of the trace of the *n*th power of the weighted adjacency matrix of the de Bruijn graph  $G_l^{(r)}$ . The correspondence is induced by that between the configurations of  $\mathcal{A}_{l+1}^{(r)}$  and the closed walks in  $G_l^{(r)}$  through the mapping  $\phi_R$  from the edge set of  $G_l^{(r)}$  into  $\mathbb{Z}_r$ . Using the correspondence, we show that there exist exactly 16 reversible elementary cellular automaton rules and give the cell sizes for which the rules are reversible. In addition, we give a sufficient condition for reversibility of the cellular automaton  $\mathcal{A}_2^{(3)}$ , and show that there exist ten reversible rules up to automorphisms.

Since our aim is to find integrable cellular automaton other than box–ball systems, we want to find as many reversible cellular automata as possible because reversibility is a necessary condition for integrability, and we will search reversible cellular automata for integrable ones. Finding sufficient conditions for reversibility of the cellular automata  $\mathcal{A}_l^{(r)}$  for greater *r* and *l* is another problem.

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