

Reversibility of Linear Cellular Automata on Cayley Trees with Periodic Boundary Condition

Chih-Hung Chang* and Jing-Yi Su

Abstract. While one-dimensional cellular automata have been well studied, there are relatively few results about multidimensional cellular automata; the investigation of cellular automata defined on Cayley trees constitutes an intermediate class. This paper studies the reversibility of linear cellular automata defined on Cayley trees with periodic boundary condition, where the local rule is given by $f(x_0, x_1, \dots, x_d) = bx_0 + c_1x_1 + \dots + c_dx_d \pmod{m}$ for some integers $m, d \geq 2$. The reversibility problem relates to solving a polynomial derived from a recurrence relation, and an explicit formula is revealed; as an example, the complete criteria of the reversibility of linear cellular automata defined on Cayley trees over $\mathbb{Z}_2, \mathbb{Z}_3$, and some other specific case are addressed. Further, this study achieves a possible approach for determining the reversibility of multidimensional cellular automata, which is known as a undecidable problem.

1. Introduction

Cellular automaton (CA) is a particular class of dynamical systems introduced by Ulam and von Neumann as a model for self-production and is widely studied in multidisciplinary areas such as physics, biology, image processing, cryptography, and pseudo-random number generation [5, 7, 9, 14, 21]. One-dimensional CA consists of the infinite lattice with finite states and a local rule; the celebrated works of Hedlund and Wolfram make a decisive impulse to the mathematical study of CA (see [10, 19] and the references therein).

A cellular automaton is called reversible if every current configuration is associated with exactly one past configuration. While the reversibility of one-dimensional CAs is elucidated [11, 16, 17], Kari indicates that the reversibility of multidimensional CAs is undecidable [12, 13]. Recently, the reversibility problem for one-dimensional cellular automata with boundary conditions has been studied [6, 8]; it is shown that a reversibly

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*Corresponding author.

linear CA is either a Bernoulli automorphism or non-ergodic [4]. Many researchers have been devoted to investigating the reversibility problem of multidimensional linear cellular automata under boundary conditions; however, there is no algorithm for determining whether a multidimensional linear cellular automaton is reversible [15, 18, 20].

The notion of CAs has been extended to the case where the underlying space is the Cayley tree of a finitely generated group or semigroup (see [1–3] and the references therein). Note that the grid \mathbb{Z}^d is the Cayley tree of the free abelian group with d generators. In other words, CAs defined on Cayley trees constitute an intermediate class in between one-dimensional and multidimensional CAs.

Some interesting phenomena are observed in reversible CA defined on Cayley trees. Figure 1.1 shows an eventually periodic orbit of a linear CA defined in the binary Cayley tree of height 5 over three symbols. Furthermore, every configuration in the orbit is symmetric.

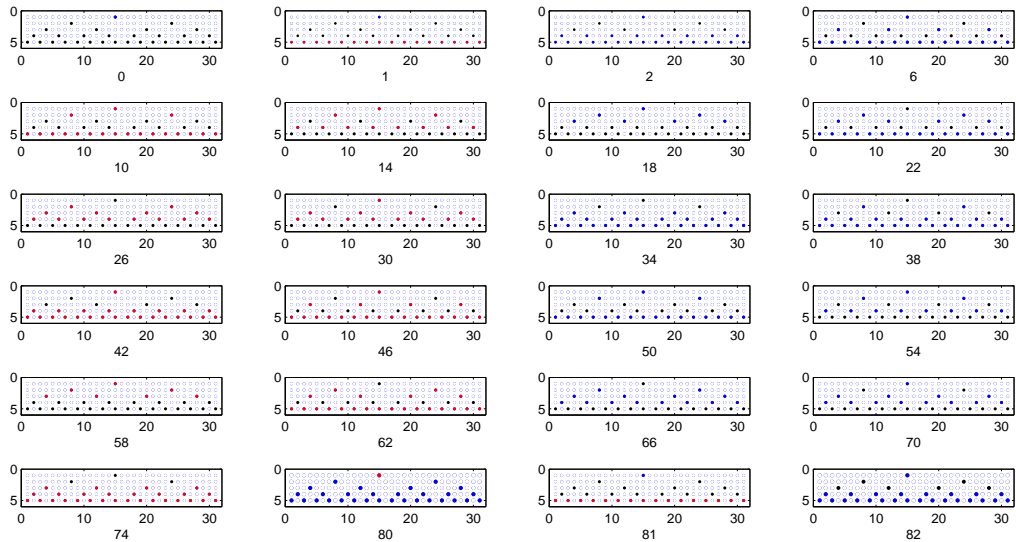


Figure 1.1: An eventually periodic orbit of CA defined on binary tree with height 5, where the local rule is given by $f(x_0, x_1, x_2) = x_0 + x_1 + x_2 \pmod{3}$. The number below each figure indicates the number of the time step; it is seen that this is an eventually periodic orbit with period 80. The color black, blue, and red represents 0, 1, and 2, respectively.

In this article, we investigate the reversibility of linear CAs defined on Cayley trees with periodic boundary condition; the matrix algebra has been used for the investigation. We define the matrix presentation of a linear CA defined on a Cayley tree of height n , and then characterize the reversibility by demonstrating an explicit formula of the determinant of its related matrix. The main difficulty comes from the exponential growth rate of the dimension of the matrix whenever n increases. Furthermore, the complete criteria for the

reversibility of linear CAs defined on Cayley trees over $\mathbb{Z}_2, \mathbb{Z}_3$, and some other conditions are addressed.

The rest of this paper is organized as follows. The upcoming section introduces some preliminaries and the reversibility of linear CAs defined in the binary Cayley tree. Section 3 elaborates the explicit criteria for the reversibility of linear CAs in some cases. Section 4 addresses the proofs of theorems stated in Section 2 while Section 5 extends all the results to general Cayley trees. Some discussions and a conclusion are given in Section 6.

2. Reversibility of CA on binary tree

This section investigates the reversibility of a cellular automaton defined in the binary Cayley tree for the clarification; the discussion extends to cellular automata defined on general Cayley trees and is illustrated later.

We start with some basic definitions of symbolic dynamics on infinite binary trees. Let $\Sigma = \{1, 2\}$ and let Σ^* be the set of words over Σ ; more specifically, $\Sigma^* = \bigcup_{n \geq 0} \Sigma^n$, where $\Sigma^n = \{w_1 w_2 \cdots w_n : w_i \in \Sigma \text{ for } 1 \leq i \leq n\}$ is the set of words of length n for $n \in \mathbb{N}$ and $\Sigma^0 = \{\epsilon\}$ consists of the empty word ϵ . An *infinite tree* t over a finite alphabet $\mathcal{A} = \{0, 1, \dots, m - 1\}$, herein $m \geq 2$, is a function from Σ^* to \mathcal{A} ; a *node* of an infinite tree is a word of Σ^* while the empty word relates to the root of the tree. Suppose that x is a node of a tree; x has two *children* x_1 and x_2 , and x is the *parent* of x_1 and x_2 . Furthermore, a node without children is called a *leaf*.

Let t be a tree and let x be a node, we refer t_x to $t(x)$ for simplicity. A subset of words $L \subset \Sigma^*$ is called *prefix-closed* if each prefix of L belongs to L . A function u defined on a finite prefix-closed subset L with codomain \mathcal{A} is called a *pattern* or *block*, and L is called the *support* of the pattern. Suppose that n is a nonnegative integer. Let $\Sigma_n = \bigcup_{k=0}^n \Sigma^k$ denote the set of words of length at most n . We say that a pattern u is a *block of height* n (or *an n -block*) if the support of u is Σ_{n-1} , denoted by $\text{height}(u) = n$.

Let $\mathcal{T} = \mathcal{A}^{\Sigma^*}$ and $\mathcal{T}_n = \mathcal{A}^{\Sigma_{n-1}}$ be the sets of infinite trees and n -blocks over \mathcal{A} , respectively, where $n \in \mathbb{N}$. $T_f: \mathcal{T} \rightarrow \mathcal{T}$ is called a cellular automaton defined on Cayley tree (TCA) \mathcal{T} with local rule f if there exists $k \in \mathbb{N}$, an ordered set $\mathcal{N} = \{y_1, \dots, y_k\} \subset \Sigma^*$, and a local map $f: \mathcal{A}^k \rightarrow \mathcal{A}$ such that $(T_f t)_x = f(t_{x\mathcal{N}})$ for all $x \in \Sigma^*$, where $x\mathcal{N} = \{xy_1, \dots, xy_k\}$ and $f(t_{x\mathcal{N}}) = f(xy_1, \dots, xy_k)$; T_f is called linear if f is linear.

This elucidation focuses on those linear TCA T_f whose local rule $f: \mathcal{A}^3 \rightarrow \mathcal{A}$ is given by $f(x_0, x_1, x_2) = bx_0 + c_1x_1 + c_2x_2 \pmod{m}$; in other words, $T_f: \mathcal{T} \rightarrow \mathcal{T}$ is defined as

$$(T_f t)_x = f(t_x, t_{x_1}, t_{x_2}) = bt_x + c_1t_{x_1} + c_2t_{x_2} \pmod{m}$$

for $x \in \Sigma^*$. A TCA with periodic boundary condition (PBC) is a cellular automaton defined on a finite tree such that the “children” of leaves is the root. More explicitly, a

linear TCA with PBC is $T_f: \mathcal{T}_n \rightarrow \mathcal{T}_n$ defined as

$$(T_f t)_x = \begin{cases} f(t_x, t_{x_1}, t_{x_2}) & \text{if } |x| \leq n - 2, \\ f(t_x, t_\epsilon, t_\epsilon) & \text{if } |x| = n - 1 \end{cases}$$

for some $n \geq 2$, where $|x|$ indicates the length of x .

To investigate the reversibility of linear TCA with PBC, we transfer the global map T_f into matrix operation. Let β be an ordered set obtained by rearranging Σ_{n-1} with respect to the lexicographical order. For each $t \in \mathcal{T}_n$, denote by $[t]_\beta \in \mathcal{A}^{2^n-1}$ the column vector of t with respect to β ; more precisely, let $\Theta: \Sigma_{n-1} \rightarrow \mathbb{N}$ be defined as

$$\Theta(x) = \begin{cases} 1 & \text{if } x = \epsilon, \\ 1 + \sum_{i=1}^k x_i 2^{k-i} & \text{if } x = x_1 \cdots x_k \in \Sigma^k, \end{cases}$$

then $[t]_\beta(i) = t_x$ for $x \in \Sigma_n$ with $\Theta(x) = i$. Let

$$T_n(i, j) = \begin{cases} b & \text{if } j = i, 1 \leq i \leq 2^n - 1, \\ c_1 & \text{if } j = 2i, 1 \leq i \leq 2^{n-1} - 1, \\ c_2 & \text{if } j = 2i + 1, 1 \leq i \leq 2^{n-1} - 1, \\ c_1 + c_2 & \text{if } j = 1, 2^{n-1} \leq i \leq 2^n - 1, \\ 0 & \text{otherwise.} \end{cases}$$

Evidently, $[T_f t]_\beta = T_n[t]_\beta \pmod{m}$, and we call T_n the *matrix presentation* of the linear TCA T_f defined on \mathcal{T}_n with PBC.

Example 2.1. Consider the case where $n = 3$, it can be verified without difficulty that

$$T_3 = \begin{pmatrix} b & c_1 & c_2 & 0 & 0 & 0 & 0 \\ 0 & b & 0 & c_1 & c_2 & 0 & 0 \\ 0 & 0 & b & 0 & 0 & c_1 & c_2 \\ c_1 + c_2 & 0 & 0 & b & 0 & 0 & 0 \\ c_1 + c_2 & 0 & 0 & 0 & b & 0 & 0 \\ c_1 + c_2 & 0 & 0 & 0 & 0 & b & 0 \\ c_1 + c_2 & 0 & 0 & 0 & 0 & 0 & b \end{pmatrix}, \quad [T_f t]_\beta = \begin{pmatrix} b & c_1 & c_2 & 0 & 0 & 0 & 0 \\ 0 & b & 0 & c_1 & c_2 & 0 & 0 \\ 0 & 0 & b & 0 & 0 & c_1 & c_2 \\ c_1 + c_2 & 0 & 0 & b & 0 & 0 & 0 \\ c_1 + c_2 & 0 & 0 & 0 & b & 0 & 0 \\ c_1 + c_2 & 0 & 0 & 0 & 0 & b & 0 \\ c_1 + c_2 & 0 & 0 & 0 & 0 & 0 & b \end{pmatrix} \begin{pmatrix} t_\epsilon \\ t_1 \\ t_2 \\ t_{11} \\ t_{12} \\ t_{21} \\ t_{22} \end{pmatrix}$$

for all $t \in \mathcal{T}_3$.

It follows immediately from the definition of $[\cdot]_\beta$ that the following are equivalent.

- (i) TCA T_f with PBC is reversible.

$$= (b + c_1 + c_2) \det \begin{pmatrix} 0 & c_1 & c_2 & 0 & 0 & 0 & 0 & -b & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & b & 0 & c_1 & c_2 & 0 & 0 & -b & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & b & 0 & 0 & c_1 & c_2 & -b & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & b & 0 & 0 & 0 & c_1 - b & c_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & b & 0 & 0 & -b & 0 & c_1 & c_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & b & 0 & -b & 0 & 0 & 0 & c_1 & c_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & b & -b & 0 & 0 & 0 & 0 & 0 & c_1 & c_2 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & b & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -b & b & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -b & 0 & b & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -b & 0 & 0 & b & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -b & 0 & 0 & 0 & b & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -b & 0 & 0 & 0 & 0 & b & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -b & 0 & 0 & 0 & 0 & 0 & b & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -b & 0 & 0 & 0 & 0 & 0 & 0 & b \end{pmatrix}$$

$$= -(b + c_1 + c_2)b^7 \det \begin{pmatrix} c_1 & c_2 & 0 & 0 & 0 & 0 & -b \\ b & 0 & c_1 & c_2 & 0 & 0 & -b \\ 0 & b & 0 & 0 & c_1 & c_2 & -b \\ 0 & 0 & b & 0 & 0 & 0 & c_1 + c_2 - b \\ 0 & 0 & 0 & b & 0 & 0 & c_1 + c_2 - b \\ 0 & 0 & 0 & 0 & b & 0 & c_1 + c_2 - b \\ 0 & 0 & 0 & 0 & 0 & b & c_1 + c_2 - b \end{pmatrix}$$

$$= (b + c_1 + c_2)(-b)^7 \det \begin{pmatrix} c_1 & c_2 & 0 & 0 & 0 & 0 & -b \\ b & 0 & 0 & 0 & 0 & 0 & -\frac{(c_1+c_2)(c_1+c_2-b)+b^2}{b} \\ 0 & b & 0 & 0 & 0 & 0 & -\frac{(c_1+c_2)(c_1+c_2-b)+b^2}{b} \\ 0 & 0 & b & 0 & 0 & 0 & c_1 + c_2 - b \\ 0 & 0 & 0 & b & 0 & 0 & c_1 + c_2 - b \\ 0 & 0 & 0 & 0 & b & 0 & c_1 + c_2 - b \\ 0 & 0 & 0 & 0 & 0 & b & c_1 + c_2 - b \end{pmatrix}$$

$$\begin{aligned}
 &= (b + c_1 + c_2)(-b)^{11} \det \begin{pmatrix} c_1 & c_2 & -b \\ b & 0 & -\frac{(c_1+c_2)(c_1+c_2-b)+b^2}{b} \\ 0 & b & -\frac{(c_1+c_2)(c_1+c_2-b)+b^2}{b} \end{pmatrix} \\
 &= -(b + c_1 + c_2)b^{11} \sum_{j=0}^3 (-1)^j (c_1 + c_2)^{3-j} b^j.
 \end{aligned}$$

3. Necessary and sufficient condition for the reversibility

This section addresses the full criteria for the reversibility of linear TCA over \mathbb{Z}_2 , \mathbb{Z}_3 , and some other case. The criteria herein focus on the binary tree for the simplicity and can be extended to general Cayley trees without difficulty.

Theorem 2.2 reveals that the necessary and sufficient conditions for a TCA T_f being reversible is

$$(b + c_1 + c_2)b^{2^n - n - 1} \sum_{j=0}^{n-1} (-1)^j (c_1 + c_2)^{n-1-j} b^j \neq 0 \pmod{m}.$$

Suppose that $m = p$ is a prime. The necessary and sufficient condition for the reversibility of T_f can be simplified as follows: T_f is reversible if and only if

- (i) $b \neq 0 \pmod{p}$;
- (ii) $b + c_1 + c_2 \neq 0 \pmod{p}$;
- (iii) $\sum_{j=0}^{n-1} (-1)^j (c_1 + c_2)^{n-1-j} b^j \neq 0 \pmod{p}$.

To ease the notation, all the evaluation are considered under modulo p in this section unless otherwise stated.

Let $g(x) = \sum_{k=0}^{n-1} (-1)^k b^k x^{n-1-k}$; elaborating the reversibility of T_f is “almost” equivalent to the discussion of the existence of the roots of $g(x)$. This section investigates the cases where $p = 2$ and $p = 3$; for each case, the reversibility of T_f is characterized explicitly. For this purpose, we assume that $b \neq 0$ in the rest of this section.

Furthermore, the reversibility of T_f for the case where $n = 2^l$ for some $l \in \mathbb{N}$ is elucidated; an interesting algebraic property is revealed.

3.1. Cases study: $p = 2$

Proposition 3.1. *T_f is reversible if and only if $b = 1$ and $c_1 + c_2 = 0$.*

Proof. Notably, we only need to consider the case where $b = 1$ when $p = 2$ since $b \neq 0$. It is seen that

$$g(x) = 1 + x + x^2 + \dots + x^{n-1}.$$

Suppose that n is even. It is easily seen that $g(x) = 0$ if and only if $x = 1$. That is, T_f is reversible if and only if $c_1 + c_2 = 0$. For the case where n is odd, $g(x)$ can be expressed as

$$g(x) = (1 + x)(1 + x^2 + x^4 + \dots + x^{n-2}) = 0 \pmod{2} \iff x = 1.$$

Both cases demonstrate that T_f is reversible if and only if $c_1 + c_2 = 0$. This completes the proof. □

Figure 3.1 illustrates a periodic orbit derived by a reversible CA defined on binary tree with height 5.

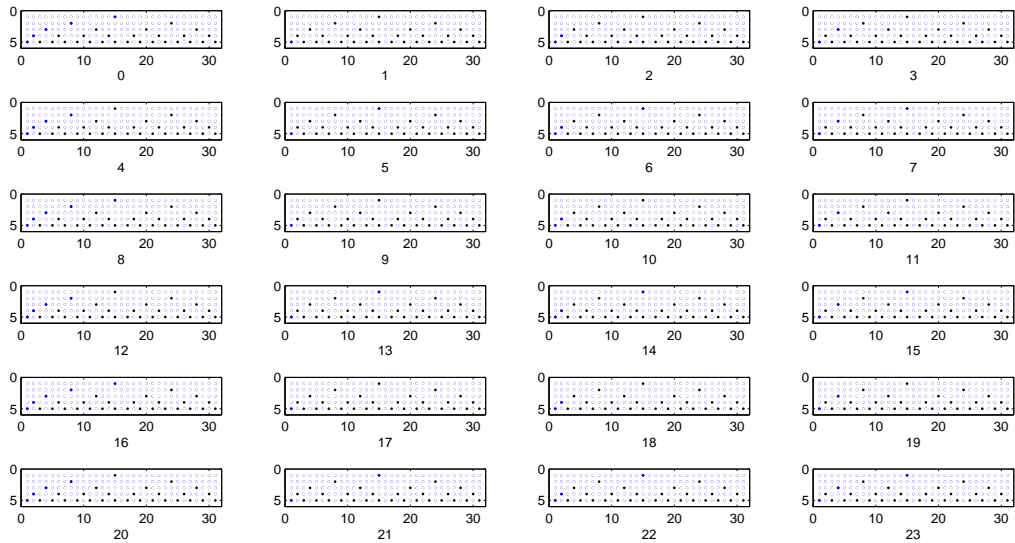


Figure 3.1: A period-8 orbit of CA defined on binary tree with height 5, where the local rule is given by $f(x_0, x_1, x_2) = x_0 + x_1 + x_2 \pmod{2}$. The color black and blue represents 0 and 1, respectively.

3.2. Cases study: $p = 3$

Recall that $b = 0$ indicates that T_f is irreversible; hence it suffices to consider the case where $b \neq 0$.

Proposition 3.2. *For the case where $p = 3$, T_f is irreversible if and only if one of the following is satisfied:*

- (1) $c_1 + c_2 = b$;
- (2) $c_1 + c_2 \neq 0$ and n is a multiple of 6;
- (3) $b + c_1 + c_2 = 0$.

Proof. Since $b \neq 0$, Fermat's Little Theorem asserts that $b^2 = 1 \pmod{3}$.

Case 1: n is even.

$$\begin{aligned} g(x) &= x^{n-1} - bx^{n-2} + b^2x^{n-3} - b^3x^{n-4} + \dots + b^{n-2}x - b^{n-1} \\ &= (x - b)(x^{n-2} + x^{n-4} + x^{n-6} + \dots + x^2 + 1) \pmod{3}. \end{aligned}$$

A straightforward examination shows that

$$x^{n-2} + x^{n-4} + x^{n-6} + \dots + x^2 + 1 = 0 \pmod{3} \iff x \neq 0 \text{ and } n = 6l$$

for some $l \in \mathbb{N}$. Therefore, $g(x) = 0 \pmod{3}$ if and only if $x = b$ or $x \neq 0$ and $n = 6l$ for some $l \in \mathbb{N}$.

Case 2: n is odd. Observe that

$$g(x) = \begin{cases} (x - 1)(x^{n-2} + x^{n-4} + \dots + x^2 + 1) & \text{if } b = 1, \\ (x + 1)(x^{n-2} + x^{n-4} + \dots + x^2 + 1) & \text{if } b = 2 \end{cases} \pmod{3}.$$

Similar to the above discussion, it follows that $g(x) = 0 \pmod{3}$ if and only if $x = b$ or $x \neq 0$ and $n = 6l$ for some $l \in \mathbb{N}$. The proof is complete. \square

3.3. Cases study: $n = 2^l$

Instead of considering the special cases $p = 2$ and $p = 3$, this subsection focuses on the case where the height of the Cayley tree is some power of 2. For this case, an algebraic property related to the reversibility of T_f is revealed.

Suppose that $n = 2^l$ for some $l \in \mathbb{N}$. It is seen that

$$\begin{aligned} g(x) &= (x - b)(x^{n-2} + b^2x^{n-4} + b^4x^{n-6} + \dots + b^{n-4}x^2 + b^{n-2}) \\ &= (x - b)(x^2 + b^2)(x^4 + b^4) \dots (x^{2^{l-1}} + b^{2^{l-1}}). \end{aligned}$$

The last equality can be demonstrated via the mathematical induction principle, thus it is omitted. The reversibility of T_f is then characterized explicitly as follows.

Proposition 3.3. *For the case where $n = 2^l$ for some $l \in \mathbb{N}$, T_f is irreversible if and only if one of the following is satisfied:*

- (1) $b + c_1 + c_2 = 0$;
- (2) $c_1 + c_2 = b$;
- (3) $p = 2^r + 1$ for some integer $r < l$ and $(c_1 + c_2)^{2^q} + b^{2^q} = 0 \pmod{p}$ for some $1 \leq q \leq r - 1$;

(4) $p \neq 2^r + 1$ for $r \geq 0$ and $(c_1 + c_2)^{2^q} + b^{2^q} = 0 \pmod p$ for some $1 \leq q \leq \gamma$, where γ is the order of the subset $A = \{2^k : k \in \mathbb{N}\}$ of \mathbb{Z}_p .

Proof. Observe that $g(x) \neq 0$ if $x = 0$ and T_f is reversible in this case; therefore, we may assume that $x \neq 0$ without loss of generality. It is obvious that the irreversibility of T_f follows from $c_1 + c_2 = b$.

Suppose that $p = 2^r + 1$ for some $r \in \mathbb{N}$. Fermat's Little Theorem asserts that $a^{2^k} = 1 \pmod p$ for all $k \geq r$ provided $a \neq 0$. It follows immediately that

$$g(x) = 2^{l-r}(x - b)(x^2 + b^2)(x^4 + b^4) \cdots (x^{2^{r-1}} + b^{2^{r-1}}).$$

Hence, $g(x) = 0$ if and only if $x = b$ or $x^{2^q} + b^{2^q} = 0 \pmod p$ for some $1 \leq q \leq r - 1$.

Suppose that the prime p cannot express as $p = 2^r + 1$ for $r \geq 0$. It can be verified that the sequence $\{2^k\}_{k \in \mathbb{N}}$ is eventually periodic. Let $A = \{2^k : k \geq 1\}$ be an ordered set with $|A| = \gamma$. There exists $\lambda \in \mathbb{N}$ such that

$$g(x) = (x - b) \left(\prod_{i=1}^{\lambda} (x^{2^i} + b^{2^i}) \right) \left(\prod_{i=\lambda+1}^{\tau} (x^{2^i} + b^{2^i}) \right)^{\kappa+1} \left(\prod_{i=\tau+1}^{\gamma} (x^{2^i} + b^{2^i}) \right)^{\kappa}$$

for some κ and τ . Evidently, $g(x) = 0$ if and only if $x = b$ or $x^{2^q} + b^{2^q} = 0$ for some $1 \leq q \leq \gamma$. This completes the proof. □

We end this section with the following two examples that illustrate the case where $p \neq 2^r + 1$ and $n = 2^l$.

Example 3.4. Suppose that $n = 2^{10}$ and $p = 7$. A routine examination infers that $x^{2^k} = x^2 \pmod 7$ if k is odd and $x^{2^k} = x^4 \pmod 7$ if k is even; that is, $A = \{2, 4\}$. It follows that

$$g(x) = (x - b)(x^2 + b^2)(x^4 + b^4) \cdots (x^{2^9} + b^{2^9}) = (x - b)(x^2 + b^2)^5(x^4 + b^4)^4.$$

Therefore, T_f is reversible if and only if (1) $b + c_1 + c_2 \neq 0$; (2) $c_1 + c_2 \neq b$ and $b \neq 0$; (3) $(c_1 + c_2)^2 + b^2 \neq 0$; (4) $(c_1 + c_2)^4 + b^4 \neq 0$.

Example 3.5. Suppose that $n = 2^{10}$ and $p = 29$. A routine examination infers that $x^{2^k} = x^4 \pmod{29}$ when $k = 3n - 1$; $x^{2^k} = x^8 \pmod{29}$ when $k = 3n$, and $x^{2^k} = x^{16} \pmod{29}$ when $k = 3n + 1$ for some natural number $n \in \mathbb{N}$. In other words,

$$\{2^k : k \geq 1\} = \{2, 4, 8, 16, 4, 8, 16, \dots\} \quad \text{and} \quad A = \{2, 4, 8, 16\}.$$

It follows that

$$\begin{aligned} g(x) &= (x - b)(x^2 + b^2)(x^4 + b^4) \cdots (x^{2^9} + b^{2^9}) \\ &= (x - b)(x^2 + b^2)(x^4 + b^4)^3(x^8 + b^8)^3(x^{16} + b^{16})^2. \end{aligned}$$

Therefore, T_f is reversible if and only if (1) $b + c_1 + c_2 \neq 0$; (2) $c_1 + c_2 \neq b$ and $b \neq 0$; (3) $(c_1 + c_2)^2 + b^2 \neq 0$; (4) $(c_1 + c_2)^4 + b^4 \neq 0$; (5) $(c_1 + c_2)^8 + b^8 \neq 0$; (6) $(c_1 + c_2)^{16} + b^{16} \neq 0$.

4. Proof of Theorem 2.2

This section contributes to the proof of Theorem 2.2; we begin with the following lemma.

Lemma 4.1. For $n \in \mathbb{N}$, let $\bar{T}_n \in \mathcal{M}_{2^{n-1}-1}(\mathbb{R})$ be a $(2^{n-1} - 1) \times (2^{n-1} - 1)$ matrix defined as

$$\bar{T}_n(i, j) = \begin{cases} -b & \text{if } j = 2^{n-1} - 1, 1 \leq i \leq 2^{n-2} - 1, \\ c_1 + c_2 - b & \text{if } j = 2^{n-1} - 1, 2^{n-2} \leq i \leq 2^{n-1} - 1, \\ b & \text{if } j = i - 1, 2 \leq i \leq 2^{n-1} - 1, \\ c_1 & \text{if } j = 2i - 1, 1 \leq i \leq 2^{n-2} - 1, \\ c_2 & \text{if } j = 2i, 1 \leq i \leq 2^{n-2} - 1, \\ 0 & \text{otherwise.} \end{cases}$$

Then $\det T_n = (-b)^{2^{n-1}-1}(b + c_1 + c_2) \det \bar{T}_n$.

Proof. Adding the k th column of T_n to the first column recursively for $k \geq 2$ derives a new matrix $T_n^{(1)}$ defined as

$$T_n^{(1)}(i, j) = \begin{cases} b & \text{if } j = i, 2 \leq i \leq 2^n - 1, \\ c_1 & \text{if } j = 2i, 1 \leq i \leq 2^{n-1} - 1, \\ c_2 & \text{if } j = 2i + 1, 1 \leq i \leq 2^{n-1} - 1, \\ b + c_1 + c_2 & \text{if } j = 1, 1 \leq i \leq 2^n - 1, \\ 0 & \text{otherwise.} \end{cases}$$

It is seen that $\det T_n = \det T_n^{(1)}$. Since every entry in the first column of $T_n^{(1)}$ is identical, substituting the entry of the first column by 1 and then adding -1 times of the 2^{n-1} th row to the other rows recursively produces a new matrix $T_n^{(2)}$ defined as

$$T_n^{(2)}(i, j) = \begin{cases} b & \text{if } j = i, 2 \leq i \leq 2^n - 1, \\ c_1 & \text{if } j = 2i, 1 \leq i \leq 2^{n-1} - 1, i \neq 2^{n-2}, \\ c_2 & \text{if } j = 2i + 1, 1 \leq i \leq 2^{n-1} - 1, \\ -b & \text{if } j = 2^{n-1}, 1 \leq i \leq 2^n - 1, i \neq 2^{n-1}, i \neq 2^{n-2}, \\ c_1 - b & \text{if } i = 2^{n-2}, j = 2^{n-1}, \\ 1 & \text{if } j = 1, i = 2^{n-1}, \\ 0 & \text{otherwise.} \end{cases}$$

Evidently, $\det T_n^{(1)} = (b + c_1 + c_2) \det T_n^{(2)}$.

After adding the k th column to the 2^{n-1} th column of $T_n^{(2)}$ recursively for $k > 2^{n-1}$, it follows immediately that the only nonzero element of k th row of $T_n^{(2)}$ is b for $k > 2^{n-1}$. Furthermore, it can be verified without difficulty that \bar{T}_n is driven from the following two steps: (i) delete the k th row and k th column of $T_n^{(2)}$ for $k > 2^{n-1}$; (ii) delete the first column and the last row. This indicates that $\det T_n^{(2)} = (-b)^{2^{n-1}-1} \det \bar{T}_n$. Hence, we derive

$$\det T_n = \det T_n^{(1)} = (b + c_1 + c_2) \det T_n^{(2)} = (b + c_1 + c_2)(-b)^{2^{n-1}-1} \det \bar{T}_n$$

and the proof is complete. □

To evaluate $\det \bar{T}_n$, we need two more lemmas.

Lemma 4.2. *Let $\alpha_3 = c_1 + c_2 - b$ and let α_n be defined recursively as*

$$\alpha_n = -\frac{\alpha_{n-1}(c_1 + c_2) + b^2}{b}, \quad n \geq 4.$$

Then

$$(4.1) \quad \alpha_n = (-1)^{n-3} \frac{\sum_{j=0}^{n-2} (-1)^j (c_1 + c_2)^{n-2-j} b^j}{b^{n-3}},$$

where $n \geq 3$.

Proof. We prove it by induction. Let $K = c_1 + c_2$; it is seen that (4.1) holds for $n = 3$. Suppose (4.1) is true when $n = m$ for some $m \geq 3$. Then

$$\begin{aligned} \alpha_{m+1} &= -\frac{\alpha_m K + b^2}{b} \\ &= -\frac{\left[(-1)^{m-3} \frac{\sum_{j=0}^{m-2} (-1)^j K^{m-2-j} b^j}{b^{m-3}} \right] K + b^2}{b} \\ &= -\frac{(-1)^{m-3} \left(\sum_{j=0}^{m-2} (-1)^j K^{m-2-j} b^j \right) K + b^{m-1}}{b^{m-2}} \\ &= (-1)^{m-2} \frac{\left(\sum_{j=0}^{m-2} (-1)^j K^{m-1-j} b^j \right) + (-1)^{m-3} b^{m-1}}{b^{m-2}} \\ &= (-1)^{m-2} \frac{\sum_{j=0}^{m-1} (-1)^j K^{m-1-j} b^j}{b^{m-2}}. \end{aligned}$$

That is, (4.1) remains to be true for $n = m + 1$. The proof is then complete by the mathematical induction principle. □

Lemma 4.3. *Suppose that $0 \leq k \leq n - 3$. Let*

$$F_n^k(i, j) = \begin{cases} \alpha_{k+3} & \text{if } i = 2^{n-k-1} - 1, j \geq 2^{n-k-2}, \\ \bar{T}_{n-k}(i, j) & \text{otherwise.} \end{cases}$$

Then $\det \bar{T}_n = (-b)^{2^{n-1}-4} \det F_n^{n-3}$, where α_k is the same as defined in Lemma 4.2.

Proof. Observe that $F_n^0 = \bar{T}_n$. For $1 \leq i \leq 2^{n-2} - 2$, adding $-c_2/b$ times of the $(2^{n-1} - (2i - 1))$ th row and $-c_1/b$ times of the $(2^{n-1} - 2i)$ th row to the $(2^{n-2} - i)$ th row of \bar{T}_n is followed by

$$\bar{T}'_n(i, j) = \begin{cases} 0 & \text{if } 2 \leq i \leq 2^{n-2} - 1, 2i - 1 \leq j \leq 2i, \\ \alpha_4 & \text{if } j = 2^{n-1} - 1, 2 \leq i \leq 2^{n-2} - 1, \\ \bar{T}_n(i, j) & \text{otherwise.} \end{cases}$$

It is seen that there is only one nonzero entry, which is b , in the k th row of \bar{T}'_n for $3 \leq k \leq 2^{n-1} - 1$. Evidently, we derive that

$$\det \bar{T}_n = \det \bar{T}'_n = (-b)^{2^{n-2}} \det F_n^1.$$

Applying similar operations to F_n^1 infers that $\det F_n^1 = (-b)^{2^{n-3}} \det F_n^2$, the desired result follows by repeating the procedure for $n - 3$ times. □

Now we are on the stage of presenting the proof of Theorem 2.2.

Proof of Theorem 2.2. Observe that

$$\begin{aligned} \det F_n^{n-3} &= \det \begin{pmatrix} c_1 & c_2 & -b \\ b & 0 & \alpha_n \\ 0 & b & \alpha_n \end{pmatrix} \\ &= -bK\alpha_n - b^3 \\ &= -bK(-1)^{n-3} \frac{\sum_{j=0}^{n-2} (-1)^j K^{n-2-j} b^j}{b^{n-3}} - b^3 \\ &= (-1)^{n-2} \frac{\sum_{j=0}^{n-2} (-1)^j K^{n-1-j} b^j + (-1)^{n-1} b^{n-1}}{b^{n-4}} \\ &= (-1)^{n-2} b^{4-n} \sum_{j=0}^{n-1} (-1)^j K^{n-1-j} b^j, \end{aligned}$$

where $K = c_1 + c_2$.

By integrating Lemmas 4.1, 4.2, and 4.3, we demonstrate that

$$\begin{aligned}
 \det T_n &= (b + c_1 + c_2)(-b)^{2^{n-1}-1} \det \bar{T}_n \\
 &= (b + c_1 + c_2)(-b)^{2^{n-1}-1}(-b)^{2^{n-1}-4} \det F_n^{n-3} \\
 &= (b + c_1 + c_2)(-b)^{2^n-5}(-1)^{n-2}b^{4-n} \sum_{j=0}^{n-1} (-1)^j K^{n-1-j}b^j \\
 &= (b + c_1 + c_2)(-b)^{2^n-n-1} \sum_{j=0}^{n-1} (-1)^j K^{n-1-j}b^j \\
 &= (b + c_1 + c_2)(-b)^{2^n-n-1} \sum_{j=0}^{n-1} (-1)^j (c_1 + c_2)^{n-1-j}b^j
 \end{aligned}$$

and this completes the proof. □

5. Reversibility of CA on general Cayley trees

This section extends results of cellular automata defined on binary tree to general Cayley trees; in other words, this section illustrates the case where $\Sigma = \{1, 2, \dots, d\}$ for some $d \geq 2$. Let $d_n = d + d^2 + \dots + d^n$; the matrix presentation T_n of CA T_f , whose local rule is given by $f(x_0, x_1, \dots, x_d) = bx_0 + \sum_{i=1}^d c_i x_i \pmod{m}$, defined on \mathcal{T}_n is defined as

$$T_n(i, j) = \begin{cases} b & \text{if } i = j, \\ c_k & \text{if } j = (i - 1)d + k + 1, 1 \leq i \leq 1 + d_{n-2}, 1 \leq k \leq d, \\ c_1 + c_2 + \dots + c_d & \text{if } j = 1, 2 + d_{n-2} \leq i \leq 1 + d_{n-1}, \\ 0 & \text{otherwise.} \end{cases}$$

The reversibility of T_f is related to the determinant of T_n being nonzero. The following theorem extends Theorem 2.2.

Theorem 5.1. *Let T_n be the matrix presentation of the linear TCA T_f defined on \mathcal{T}_n with periodic boundary condition. Then*

$$\det T_n = (-1)^{d_{n-1}-n+1}(b + c)b^{d_{n-1}-n+1} \sum_{j=0}^{n-1} (-1)^j c^{n-1-j}b^j,$$

where $c = c_1 + \dots + c_d$.

Similar to the proof of Theorem 2.2, we need several lemmas for the demonstration of Theorem 5.1.

Lemma 5.2. For $n \in \mathbb{N}$, let \bar{T}_n be defined as

$$\bar{T}_n(i, j) = \begin{cases} -b & \text{if } j = 1 + d_{n-2}, 1 \leq i \leq 1 + d_{n-3}, \\ c_1 + c_2 + \dots + c_d - b & \text{if } j = 1 + d_{n-2}, 2 + d_{n-3} \leq i \leq 1 + d_{n-2}, \\ b & \text{if } j = i - 1, 2 \leq i \leq 1 + d_{n-2}, \\ c_k & \text{if } j = (i - 1)d + k, 1 \leq i \leq 1 + d_{n-3}, 1 \leq k \leq d, \\ 0 & \text{otherwise.} \end{cases}$$

Then $\det T_n = (-b)^{d^{n-1}-1}(b + c_1 + c_2 + \dots + c_d) \det \bar{T}_n$.

Proof. The proof is similar to the discussion of proof for Lemma 4.1, thus we only sketch the main steps herein.

Adding the k th column of T_n to the first column recursively for $k \geq 2$ derives a new matrix $T_n^{(1)}$ defined as

$$T_n^{(1)}(i, j) = \begin{cases} b & \text{if } i = j, 2 \leq i \leq 1 + d_{n-1}, \\ c_k & \text{if } j = (i - 1)d + k + 1, 1 \leq i \leq 1 + d_{n-2}, 1 \leq k \leq d, \\ b + c_1 + \dots + c_d & \text{if } j = 1, 1 \leq i \leq 1 + d_{n-1}, \\ 0 & \text{otherwise.} \end{cases}$$

It is seen that $\det T_n = \det T_n^{(1)}$. Since each entry in the first column of $T_n^{(1)}$ is identical, replacing the entry in the first column by 1 and adding the -1 times of the $(d_{n-2} + 2)$ th row to the other rows recursively produce a new matrix $T_n^{(2)}$ defined as

$$T_n^{(2)}(i, j) = \begin{cases} b & \text{if } j = i, 2 \leq i \leq 1 + d_{n-1}, \\ c_1 & \text{if } j = (i - 1)d + 2, 1 \leq i \leq 1 + d_{n-2}, i \neq 2 + d_{n-3}, \\ c_k & \text{if } j = (i - 1)d + k + 1, 1 \leq i \leq 1 + d_{n-2}, 2 \leq k \leq d, \\ -b & \text{if } j = 2 + d_{n-2}, 1 \leq i \leq 1 + d_{n-1}, i \neq 2 + d_{n-3}, i \neq 2 + d_{n-2}, \\ c_1 - b & \text{if } i = 2 + d_{n-3}, j = 2 + d_{n-2}, \\ 1 & \text{if } j = 1, i = 2 + d_{n-2}, \\ 0 & \text{otherwise.} \end{cases}$$

It follows immediately that $\det T_n = \det T_n^{(1)} = (b + c_1 + c_2 + \dots + c_d) \det T_n^{(2)}$.

Furthermore, after adding the $(3 + d_{n-2})$ th, $(4 + d_{n-2})$ th, \dots , $(1 + d_{n-1})$ th column to the $(2 + d_{n-2})$ th column of $T_n^{(2)}$, it can be verified without difficulty that $\det T_n^{(2)} = (-b)^{d^{n-1}-1} \det \bar{T}_n$. Evidently,

$$\det T_n = (b + c_1 + c_2 + \dots + c_d) \det T_n^{(2)} = (-b)^{d^{n-1}-1}(b + c_1 + c_2 + \dots + c_d) \det \bar{T}_n.$$

This completes the proof. □

Lemma 5.3. Let $\alpha_3 = c_1 + c_2 + \dots + c_d - b$ and let α_n be defined recursively as

$$\alpha_n = -\frac{\alpha_{n-1}(c_1 + c_2 + \dots + c_d) + b^2}{b} \quad \text{for } n \geq 4.$$

Then

$$\alpha_n = (-1)^{n-3} \frac{\sum_{j=0}^{n-2} (-1)^j (c_1 + c_2 + \dots + c_d)^{n-2-j} (b)^j}{b^{n-3}}.$$

Proof. The proof is analogous to the proof of Lemma 4.2, hence it is omitted. □

Lemma 5.4. For $0 \leq k \leq n - 3$, let

$$F_n^k(i, j) = \begin{cases} \alpha_{k+3} & \text{if } i = d^{n-k-1} - 1, j \geq d^{n-k-2}, \\ \bar{T}_{n-k}(i, j) & \text{otherwise.} \end{cases}$$

Then $\det \bar{T}_n = (-b)^{\sum_{i=2}^{n-2} d^i} \det F_n^{n-3}$.

Proof. Notably, $F_n^0 = \bar{T}_n$. Analogous to the elaboration of the proof of Lemma 4.3, observe that

- (i) adding $-c_d/b$ times of the $(1 + d_{n-2})$ th row, $-c_{d-1}/b$ times of the d_{n-2} th row, \dots , $-c_1/b$ times of the $(2 + d_{n-2} - d)$ th row to the $(1 + d_{n-3})$ th row;
- (ii) adding $-c_d/b$ times of the $(1 + d_{n-2} - d)$ th row, $-c_{d-1}/b$ times of the $(d_{n-2} - d)$ th row, \dots , $-c_1/b$ times of the $(2 + d_{n-2} - 2d)$ th row to the d_{n-3} th row;
- (iii) repeating similar operations above until adding $-c_d/b$ times of the $(1 + d_{n-2} - d(d - 1))$ th row, $-c_{d-1}/b$ times of the $(d_{n-2} - d(d - 1))$ th row, \dots , $-c_1/b$ times of the $(2 + d_{n-2} - d^2)$ th row to the $(2 + d_{n-3} - d)$ th row;

it follows immediately that $\det \bar{T}_n = (-b)^{d^{n-2}} \det F_n^1$. Continuing similar steps recursively $(n - 3)$ times derive that $\det \bar{T}_n = (-b)^{\sum_{i=2}^{n-2} d^i} \det F_n^{n-3}$. This completes the proof. □

Proof of Theorem 5.1. It is seen that

$$\begin{aligned} \det F_n^{n-3} &= \det \begin{pmatrix} c_1 & c_2 & \dots & c_d & -b \\ b & 0 & & 0 & \alpha_n \\ 0 & b & & \vdots & \alpha_n \\ \vdots & \vdots & \ddots & 0 & \vdots \\ 0 & 0 & & b & \alpha_n \end{pmatrix} \\ &= (-b)^{d-1} \det \begin{pmatrix} c_1 & -\frac{(c_2+c_3+\dots+c_d)\alpha_n+b^2}{b} \\ b & \alpha_n \end{pmatrix} \end{aligned}$$

$$\begin{aligned}
 &= (-b)^{d-1}(c\alpha_n + b^2) \\
 &= (-b)^{d-1} \left[(-1)^{n-3} \frac{\sum_{j=0}^{n-2} (-1)^j c^{n-1-j} b^j}{b^{n-3}} + b^2 \right] \\
 &= (-b)^{d-1} \left[(-1)^{n-3} \frac{\sum_{j=0}^{n-2} (-1)^j c^{n-1-j} b^j + (-1)^{n-1} b^{n-1}}{b^{n-3}} \right] \\
 &= (-b)^{d+2-n} \sum_{j=0}^{n-1} (-1)^j c^{n-1-j} b^j,
 \end{aligned}$$

where $c = c_1 + c_2 + \dots + c_d$.

Combining Lemmas 5.2, 5.3, and 5.4 infers that

$$\begin{aligned}
 \det T_n &= (-b)^{d^{n-1}-1} (b+c) \det \bar{T}_n \\
 &= (b+c)(-b)^{d^{n-1}-1} (-b)^{\sum_{i=2}^{n-2} d^i} \det F_n^{n-3} \\
 &= (b+c)(-b)^{(\sum_{i=2}^{n-1} d^i)-1} (-1)^{n-3} (-b)^{d-1} \left[\sum_{j=0}^{n-1} (-1)^j c^{n-1-j} (b)^j \right] b^{3-n} \\
 &= (-1)^{n-3} (b+c)(-b)^{(\sum_{i=1}^{n-1} d^i)-2} b^{3-n} \sum_{j=0}^{n-1} (-1)^j c^{n-1-j} b^j \\
 &= (-1)^{n-3} (b+c)(-b)^{(\sum_{i=1}^{n-1} d^i)-2} b^{3-n} \sum_{j=0}^{n-1} (-1)^j c^{n-1-j} b^j \\
 &= (-1)^{(\sum_{i=1}^{n-1} d^i)+1-n} (b+c) b^{(\sum_{i=1}^{n-1} d^i)+1-n} \sum_{j=0}^{n-1} (-1)^j c^{n-1-j} b^j.
 \end{aligned}$$

The desired result then follows. □

From those cases we studied in Section 3, it is seen that the reversibility of T_f depends on not only the parameters in the local rule but also n and m . The reversibility for the general cases is much more complicated and cannot be completely investigated by only finitely many cases. More explicitly, Section 3 reveals that the reversibility for the cases where $p = 2$ and $p = 3$ are totally different. A reversible TCA for $p = 2$ is irreversible for $p = 3$. Hence, we skip the case study for the compactness of this paper.

6. Conclusion and discussion

This elucidation demonstrates that the reversibility problem of linear cellular automata defined on Cayley trees with periodic boundary condition relates to solving a polynomial derived from a recurrence relation and the coefficients of the local rules; as an example, the complete criteria of the reversibility of cellular automata over \mathbb{Z}_2 , \mathbb{Z}_3 , and some other

specific case are addressed. Note that the grid of \mathbb{Z}^d is a Cayley graph of free abelian group with d generators; this makes the present study a possible approach for determining the reversibility of multidimensional cellular automata, which is known as an undecidable problem. The related exploration remains interesting.

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Chih-Hung Chang and Jing-Yi Su

Department of Applied Mathematics, National University of Kaohsiung, Kaohsiung
81148, Taiwan

E-mail address: chchang@nuk.edu.tw, snowinds127@gmail.com