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# Boundary problems in cellular automata for topological insulators

D P Fedchenko<sup>1,2</sup>, V V Novikov<sup>1,3</sup> and I V Timofeev<sup>2,1</sup>

<sup>1</sup> Siberian Federal University, Krasnoyarsk, 660041, Russia

<sup>2</sup> Kirensky Institute of Physics, Federal Research Center KSC SB RAS, Krasnoyarsk, 660036, Russia

<sup>3</sup> E-mail: work\_vladimir\_novikov@mail.ru

**Abstract.** In physics, a topological insulator is a material that simultaneously exhibits the properties of a conductor on the surface and an insulator in the bulk. An abstract model of a two-dimensional topological insulator is described in terms of tricolour cellular automata and excitations of a topological insulator are classified.

## 1. Introduction

The finite automata have been objects of mathematical research at the Soviet Union and abroad for about the same time [see, for example, 1–2]. Cellular automata have been widely discussed since 1970, when the British mathematician John Horton Conway devised the Game of Life. Later on, Stephen Wolfram described a class of elementary cellular automata. After that, it became clear that the Game of Life is just one rule, probably the most outstanding, from  $2^{2^8}$  possible rules for a two-dimensional cellular automaton with a Moore neighbourhood. Cellular automata are used in the simulation of ecosystems and population dynamics. The coloring of shells of some marine molluscs resembles rule 30 of a one-dimensional cellular automaton. Cellular automata are used in attempts to design processors and create the data encryption methods. The Wolfram code is a universal and highly compact way to specify a cellular automaton [3, 4]. The use of various cellular automata in solving specific problems was reviewed in [5].

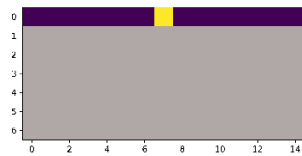
Let us consider a one- or two-dimensional homogeneous structure. The case in hand is an infinite line or a field of identical cells filled with zeros and ones (the initial state of a cellular automaton). We introduce an abstract clock generator into the system and, at each clock cycle, specify a conversion rule unified for all cells. In the Stephen Wolfram's studies, such structures are called the class of elementary cellular automata. We consider one- and two-dimensional (with the Neumann and Moore neighbourhoods) elementary cellular automata. The rules of a one-dimensional cellular automaton are specified in the form of eight-dimensional binary vectors (figure 1).



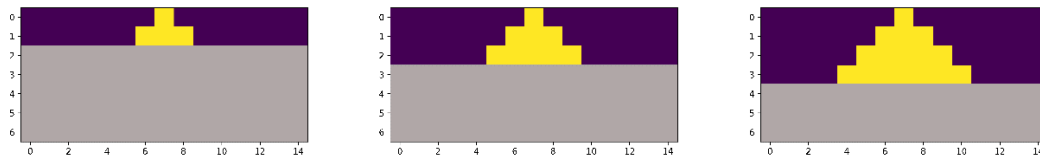
**Figure 1.** Ones are colored in yellow and zeros, in purple. The three upper cells will be called the neighbourhood. The figure illustrates rule (0, 1, 1, 1, 1, 1, 1, 1) equal to 254 in decimal notation.



The dynamics of a cellular automaton in accordance with rule 254 is presented in figures 2 and 3.

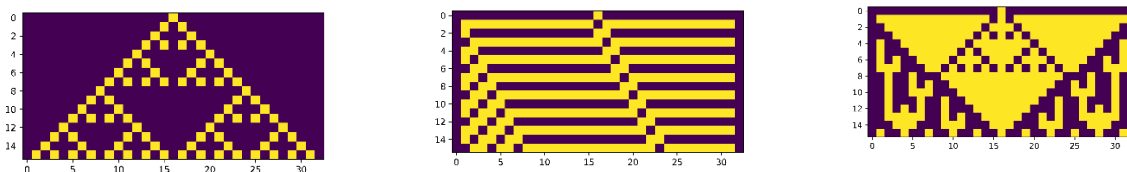


**Figure 2.** Initial state of the cellular automaton.



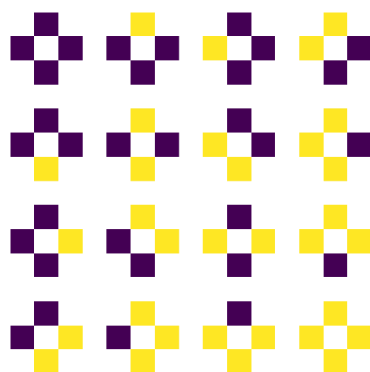
**Figure 3.** Clock cycles of the cellular automaton operation in accordance with rule 254. The neighbourhood of the cell paints the latter from the bottom according to the scheme shown in figure1.

Since the investigated range of changes in cellular automata is limited, the images in figure 4 contain a boundary defect. This defect exists in rule 26 (and in all the even rules), but we cannot see it; in the odd rules, it significantly distorts the picture. This effect can certainly be eliminated by programming tools. In our opinion, however, the theory of discrete boundary value problems can be developed here.



**Figure 4.** Examples of visualization of the draw\_rule (length, rule\_number) function. Rules 26, 59, and 165 (from left to right).

Two-dimensional cellular automata are built in a similar way. The four neighbors (above, below, left, and right) of a cell will be called its Neumann neighborhood. The rules are set by a 16-dimensional vector, according to figure5. The eight neighbors sharing an edge or a vertex with the specified cell will be called its Moore neighborhood. The Game of Life is a cellular automaton with a Moore neighborhood.

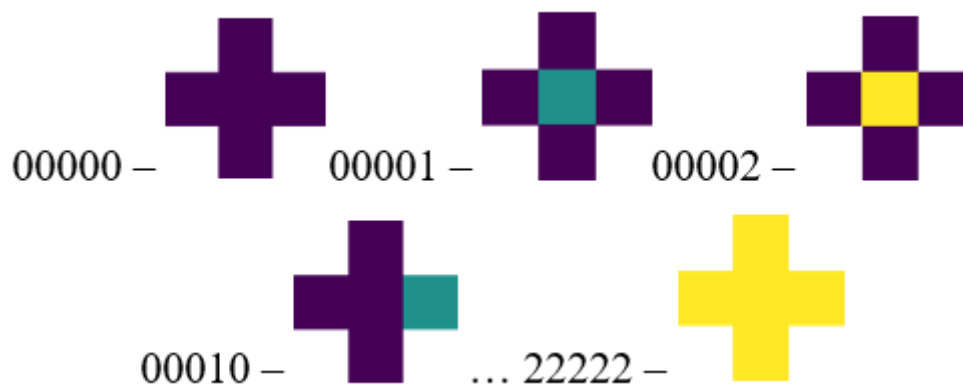


**Figure 5.** Punctured Neumann neighbourhood. There are 16 components in total in the vector of zeros and ones. Components are numbered top-down and left-to-right.

### 2. Abstract Topological Insulator

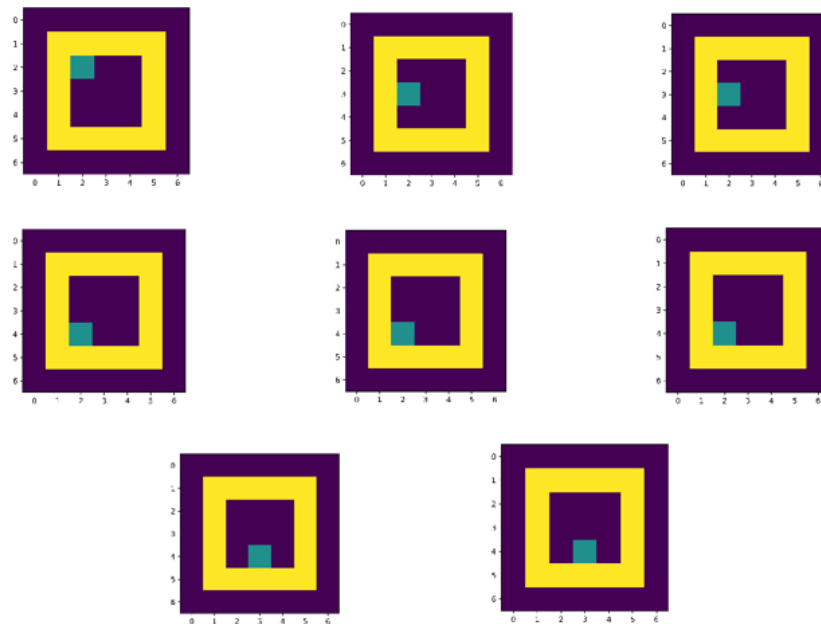
When building a model of an abstract topological insulator [6–10], we came to the consideration of tricolour cellular automata with a varying rule with period 4. The Neumann neighbourhood for such a cellular automaton is shown in figure 6.

**Rule 1** =  
 87189642485960958202911070585860771696858196300629529285884717025707245184955461514567350134642761960475397463135221,  
**Rule 2** =  
 87189642485960958202911070585860771696865629006937516856646420535307083748847009511688466704807114187492178155124653,  
**Rule 3** =  
 871896424859609582029110705858607716968657588792402221282547761642305110322715914450484937842398638240540827194153814,  
**Rule** =  
 87189642485960958202911070585860771696865758879493973628716181482036815078820525046538331816246773325439025350595533.



**Figure 6.** Neumann neighbourhood for a tricolour cellular automaton. State 0 is coloured in violet; state 1, in cyan; and state 2, in yellow. Ordering of  $3^5$  states of the neighbourhood.

Figure 7 shows the structure of an abstract topological insulator. According to the definition of a topological insulator, (i) the signal propagates along the surface and (ii) the signal that does not hit the boundary runs into a cyclic path; i.e., in the bulk, the cellular automaton exhibits the properties of an insulator. These two properties are invariant relative to the topology-preserving boundary violations.



**Figure 7.** Empty cells (0) are coloured in purple, cells with one (1) are coloured in blue, and the boundary (2), in yellow. The signal that hits the boundary runs along it and, once inside an empty area, moves through a cycle of four cells (is isolated). In some clock cycles, the signal may remain in place. The pictures are viewed top-down and left-to-right.

We have implemented an abstract topological insulator in terms of a tricolour cellular automaton with the periodic rules.

### 3. Definitions and Classification

**Definition 1.** Two cells are called connected if their values differ from 2 and, at the same time, they have a common side or a common connected cell.

**Definition 2.** An island is a collection of connected cells.

We limit the further consideration to finite islands.

**Definition 3.** A cell with a value different from 2 is called boundary (irregular) if there are cells 2 (the cells with a value of 2) in its Neumann neighbourhood.

**Definition 4.** A particle is a state of a cell with value 1.

**Definition 5.** Displacement of a particle is the transfer of the value (state) of a cell from the Neumann neighbourhood to its center in one clock tick.

**Definition 6.** A clock particle is the position of a particle on a certain clock tick.

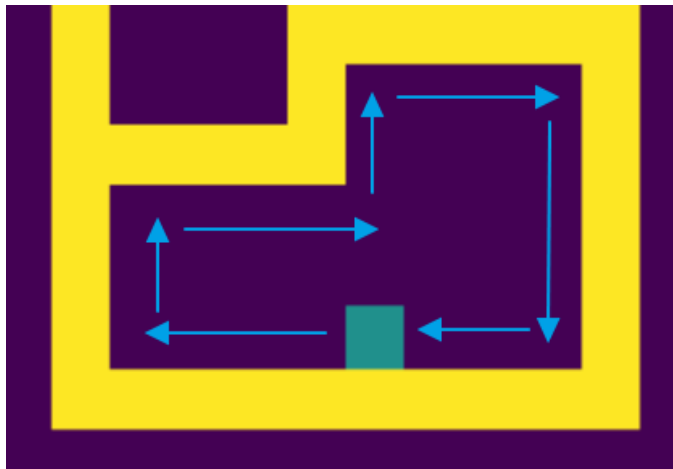
Note that a cell and a particle are related algorithmically as a variable and its value. Physically, cells, particles, and clock particles are related as space, matter, and events.

In addition, note that the states of a cell with 0 (holes) move in the same way and in the same direction as the particles.

**Definition 7.** A particle is called boundary (irregular) if the length of its clock cycle (see below) is not 4. This definition contains the classification of particles.

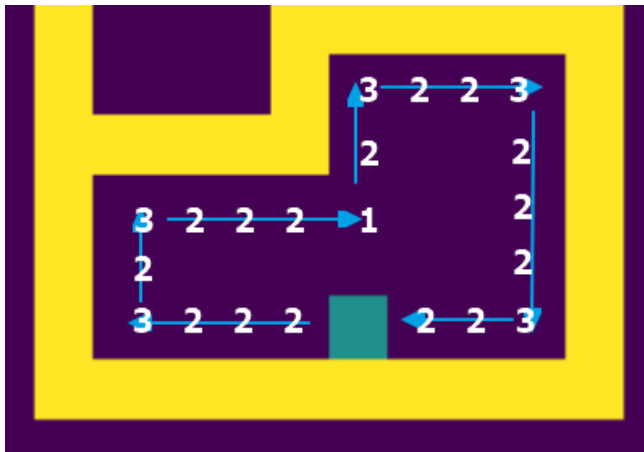
**Definition 8.** A particle path is a graph with cells as the vertices and particle displacements as edges.

The path of a boundary particle can contain regular cells. The paths of regular particles can pass through the boundary cell.



**Figure 8** A particle path along the boundary of a cellular automaton.

**Definition 9.** The clock path (world line) of a particle is a graph of the clock particles of this particle.



**Figure 9** The clock path of a particle in cellular automaton.

Obviously, the paths of different particles can intersect in common cells.

**Lemma 1.** The clock paths of different particles do not intersect.

*Proof.* We prove Lemma 1 by contradiction. Let two different clock paths have a common clock particle. Then, further clock particles will also coincide due to the complete determinism of the process. The previous clock particles will coincide for the same reason. Consequently, the clock paths coincide and we arrive at the contradiction. □

Lemma 1 is a consequence of the theorem of uniqueness of the clock path for an arbitrary clock particle.

**4. Properties of the particle in the model of an abstract topological insulator (ATI):**

- The number of particles is conserved in the model. This property is a direct consequence of Lemma 1.
- The number of clock paths is equal to the number of cells on the island, since one and only one clock path passes through each cell at a fixed clock *tick*.
- Due to the finiteness of the island, the particle moves through the cycle. The number of clock particles on the island is finite. By contradiction, every clock path crosses itself and therefore returns to the initial clock particle. A clock path can be called a clock cycle.

**Theorem 1.** The number of clock ticks during which the particle remains in the cell does not exceed the number of cells 2 in the Neumann neighborhood plus one, or the cell is bounded on four sides.

Proof. The proof is performed by the exhaustive search. The first case is a regular cell. The number of cells 2 in the neighborhood is 0. The number of clock ticks is 1, since, in the first clock cycle, the particle inevitably leaves the cell. The second case is four cells 2 in the Neumann neighborhood. This is a one-cell island. The theorem is true. In the last case, the Neumann neighborhood contains both cells 2 and non-cells 2. A particle hits a cell on the clock tick and the latter is added with the number of clock ticks equal to the number of cells 2 in the neighborhood. This number is no more than the total number of cells 2 in the neighborhood. The theorem is true. Theorem 1 is illustrated in figure 7.  $\square$

A consequence of the above classification is the correspondence of the described cellular automaton and a topological insulator. Regular particles with a clock cycle length of 4 remain within four neighboring cells and correspond to an insulator in the bulk of the island. The boundary particles can have an arbitrarily long path and correspond to a conductor at the island boundary. Thus, both defining properties of a topological insulator (nonconductive and conductive) are preserved, which confirms the correspondence.

### Acknowledgments

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