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Two extensions of exact non-equilibrium steady states of a boundary driven cellular automaton

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Abstract. Recently Prosen and Mejía-Monasterio (*J. Phys. A: Math. Theor.* **49** (2016) 185003) obtained exact nonequilibrium steady states of an integrable and reversible cellular automaton driven by some stochastic boundary conditions. In this paper, we explore the possible extensions of their method by generalizing the boundary conditions. As the result, we find two cases where such an extension is possible. One is the case where a special condition is satisfied in a generalized boundary condition. The other is obtained by considering a conserved quantity as energy and boundaries as heat reservoirs. The latter includes the original solution as the special case. Properties of the both solutions are discussed.

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1. Introduction

A cellular automaton (CA) is a discrete dynamical system composed of regularly ordered cells. The state of each cell takes values on a finite set. The cells simultaneously update their states in discrete time according to a deterministic local rule. Since Wolfram's work [1], CAs are not only studied in traditional computation theory and mathematics but also widely applied in various fields of science including fluid mechanics [2], reaction-diffusion systems [3], and integrable dynamical systems [4].

One of the authors studied one-dimensional reversible CA of the form [5, 6, 7]

$$x_i^{t+1} = f(x_{i-1}^t, x_i^t, x_{i+1}^t) \oplus x_i^{t-1}, \tag{1}$$

where i and t denote integers representing cell and time, respectively, $x_i^t \in \{0, 1\}$ means the state of cell i at time t, and \oplus the exclusive OR operation; $0 \oplus 0 = 1 \oplus 1 = 0$ and $0 \oplus 1 = 1 \oplus 0 = 1$. This CA is time-reversal invariant because the time-reversed evolution follows the same rule as

$$x_i^{t-1} = f(x_{i-1}^t, x_i^t, x_{i+1}^t) \oplus x_i^{t+1}. \tag{2}$$

This type of CA is the second-order variant of Wolfram's elementary CA, so is called elementary reversible CA (ERCA). Each rule is referred to as Wolfram's code $\sum_{x,y,z=0,1} f(x,y,z) 2^{4x+2y+z}$ appended by an 'R'. For example, if f(000) = f(010) = 0and f(x, y, z) = 1 for other configurations, the rule is called 250R. Due to the discrete nature of CA, the time-reversal invariance readily means the preservation of phase volume like Liouville's theorem in statistical mechanics. Thus, if an ERCA has an additive conserved quantity, we can define time-invariant Gibbs measure by considering the conserved quantity as energy. A necessary and sufficient condition for a CA to have an additive conserved quantity was derived and it turns out that some rules in ERCA certainly have such conserved quantities [8]. Thus ergodic properties and phase space structures are examined for some rules [5, 6]. Moreover, we can attach a heat reservoir to either end of the system by devising some stochastic update rule for the cell at the end. When the reservoirs at the left and right ends have different temperatures, there occurs transport of energy. It was numerically revealed that rule 90R shows ballistic transport, while rule 26R shows diffusive motion of energy, which leads to the Green-Kubo formula for thermal conductivity [7].

Recently, Prosen and Mejía-Monasterio [9] proposed a similar reversible cellular-automaton model with stochastic boundary conditions which represents chemical baths for absorbing and emitting particles. Their model is based on rule 54 (RCA54) presented by Bobenko et al [10] which is defined on a one-dimensional zigzag chain. At first glance, ECA54 is different from ERCA, but it is related to rule 250R in ERCA as we will see afterwards. Prosen and Mejía-Monasterio not only proved the existence and uniqueness of a nonequilibrium steady state (NESS) for RCA54, but also explicitly obtained an exact solution using a form of matrix product ansatz called the patch state ansatz. This is the first time that an exact NESS is obtained for nontrivial boundary driven CA models. Prosen and Buča [11] introduced a different kind of matrix product ansatz

to discuss the NESS and decay modes for the same CA with two kinds of boundary conditions; One is the same as in [9] and is called the Bernoulli driving in [11], and the other is called the conditional boundary driving.

It is worth studying how far the method, the model and the boundary conditions can be generalized. In this paper, we explore the possibility of extending Prosen and Mejía-Monasterio's method by devising novel boundary conditions for the same model as in [11]. As the result, we find two generalizations as follows. One is the case where parameters for absorption and emission satisfy a special relation, while probabilities for virtual cells are generalized. This is essentially equivalent to the conditional boundary driving in [11]. However, we provide an exact solution in a different form from that given in [11] using the patch state ansatz. The other generalization is obtained by employing the boundary conditions similar to that for ERCA. In fact, it turns out that this boundary condition includes both the conditional boundary driving and Bernoulli boundary driving as special cases. We explain the former in the following section and the latter in Section 3. Section 4 is devoted to summary and discussion.

2. Boundary driven cellular automaton model

2.1. Definitions

Though our model is the same as that in [9] except the boundary conditions, we give a detailed account on the model to make the manuscript self-contained.

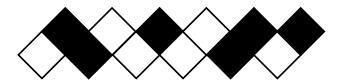


Figure 1. Illustration of a configuration of our system composed of 12 diamondshaped cells. Each cell takes value 0 (white) or 1 (black). This figure represents the configuration 011001001101.

RCA54 is a one-dimensional discrete system which consists of cells connected zigzag as in Figure 1. Each cell takes value 0 or 1. For simplicity, we assume that the number of cells n is even. The value of each cell at the next time step is determined by the following rules:

$$s_{2k}^{t+1} = \chi(s_{2k-1}^t, s_{2k}^t, s_{2k+1}^t)
 s_{2k+1}^{t+1} = \chi(s_{2k}^{t+1}, s_{2k+1}^t, s_{2k+2}^{t+1}),$$
(3)

$$s_{2k+1}^{t+1} = \chi(s_{2k}^{t+1}, s_{2k+1}^t, s_{2k+2}^{t+1}), \tag{4}$$

where $s_i^t \in \mathbb{Z}_2 = \{0, 1\}$ is a value of the *i*-th cell at time t and $\chi : \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2 \to \mathbb{Z}_2$ is defined as

$$\chi(s, s', s'') = s \oplus s' \oplus s'' \oplus ss''. \tag{5}$$

This rule is illustrated in Figure 2. Equation (5) has the following property

$$\chi(s, s', s'') = t \qquad \Leftrightarrow \qquad \chi(s, t, s'') = s',$$
(6)

which means that the CA is time-reversal invariant. Wolfram code for this χ is 54, so this CA is called RCA54. It should be noticed that there is no relation to Wolfram's elementary CA or ERCA with the same code number.

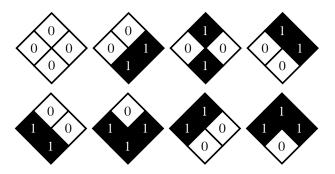


Figure 2. All patterns of (5). The value of the bottom cell is determined from the values of the top, left, and right cells.

In RCA54, cells with value 1 look like trajectories of particles moving from side to side with velocity ± 1 (see Figure 3). The time-reversal symmetry (6) is similar to that of motion in Newtonian mechanics.

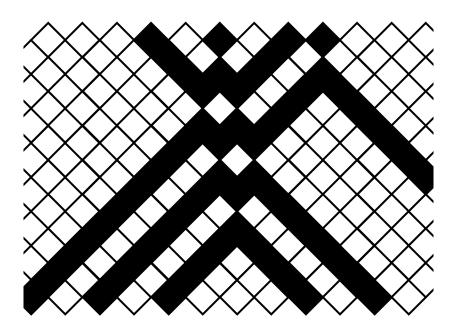


Figure 3. An example of trajectory in RCA54, where the initial configuration is given by Figure 1. All cells outside the figure are assumed to be 0. Value 1 colored black moves to left or right with velocity ± 1 until collision occurs. When two particles collide, they shifts to the next lower cell and then move away separately.

In finite systems of RCA54, some boundary condition is necessary to determine values of the boundaries i=1 and n, which cannot be determined by (3) or (4) only. For that purpose, we consider virtual cells i=0 and n+1 outside of the both ends of the system. Value of the 0th cell is given as $s_0^{t+1}=0$ with probability ζ , and $s_0^{t+1}=1$ with $1-\zeta$. On the other hand, value of the (n+1)-st cell is given as $s_{n+1}^{t+1}=0$ with probability η , and $s_{n+1}^{t+1}=1$ with $1-\eta$. Then, we can apply the rule and determine the next time values of both end cells (Figure 4). This is a generalization from [9], where only the case $\zeta=\eta=1/2$ is considered.

Moreover, we take into account emission and absorption of particles at the boundaries as follows. If $s_1^t = 0$ at time t, change it to $s_1^t = 1$ with probability α , which corresponds to emission. On the other hand, if $s_1^t = 1$ at time t, change it to $s_1^t = 0$ with probability β , which corresponds to absorption (Figure 5).

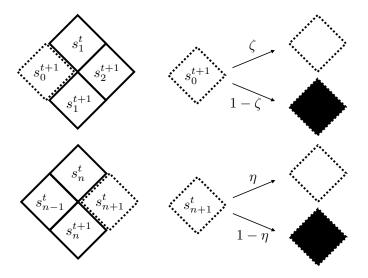


Figure 4. Boundary conditions to give s_1^{t+1} and s_n^{t+1} . Make the virtual cell on the outside so that the rule (5) can be applied. The two parameters are in the range $0 < \zeta, \eta < 1$.

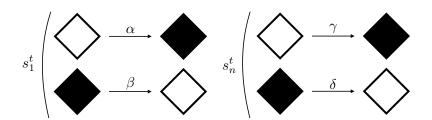


Figure 5. Boundary conditions corresponding to particle absorption/emission, stochastically generate or annihilate the value 1 at the end cells 1, n. The four parameters are in the range $0 < \alpha, \beta, \gamma, \delta < 1$.

Thus, in RCA54, the bulk is deterministically and the boundary is stochastically developed temporally. A configuration at time t is represented by a binary sequence

 $s^t = s_1^t s_2^t \cdots s_n^t$. Because each configuration corresponds one-to-one to the binary number of n digits, the total number of configurations is 2^n .

2.2. Master equation

Let p_s^t be the probability of taking configuration s at time t. The state of the system at time t is given by state vector $\underline{p}^t = (p_0^t, p_1^t, \dots, p_{2^n-1}^t)$ which evolves in time according to the master equation of the form $p^{t+1} = Up^t$, or

$$p_{\mathbf{s}}^{t+1} = \sum_{\mathbf{s}'} U_{\mathbf{s}\mathbf{s}'} p_{\mathbf{s}'}^t, \tag{7}$$

where $U = (U_{ss'})$ is the $2^n \times 2^n$ transition matrix. We want to find the $2^n \times 2^n$ transition matrix from time t to t + 1, U.

As stated in the previous subsection, the time evolution of RCA54 is divided into two steps: (i) values of even-numbered cells except cell n are determined by the rule (3), and that of cell n by the boundary condition, and (ii) values of odd-numbered cells except cell 1 are determined by the rule (4), and that of cell 1 by the boundary condition. Let the configuration at time t be $\mathbf{s} = s_1 \cdots s_n$ and that at time t+1 be $\mathbf{u} = u_1 \cdots u_n$. Then, step (i) changes configuration \mathbf{s} to $s_1 u_2 s_3 u_4 \cdots u_n$, which is transformed into \mathbf{u} by step (ii) (see Figure 6). It is noted that in step (i) u_{2k} is determined only from the three values s_{2k-1} , s_{2k} , s_{2k+1} and u_n is probabilistically chosen depending on s_{n-1} and s_n . Each transition is represented by small transition matrices.

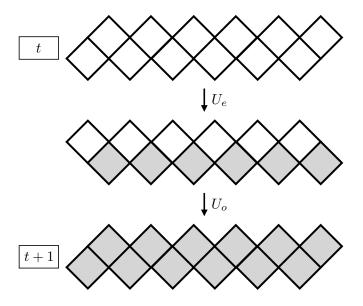


Figure 6. Separation of time evolution. U_e and U_o are transition matrices corresponding to steps (i) and (ii) respectively.

Transition from $s_{2k-1}s_{2k}s_{2k+1}$ to $s_{2k-1}u_{2k}s_{2k+1}$ is given by (3). Interpreting this transition as a 3-digit binary number to a 3-digit binary number, the local transition

matrix is written using the following 8×8 matrix

or tensor

$$P_{uu'u''|ss's''} = \delta_{us}\delta_{u'\chi(s,s',s'')}\delta_{u''s''}.$$
(9)

The rows and columns are labeled ss's'' (in order of 000, 001, 010, 011, 100, 101, 110, 111). The same transition matrix is also utilized in step (ii).

The transition matrix at the boundary is obtained as follows. The absorption/emission part is expressed by 2×2 matrices that acts only on the end cells 1 or n, as

$$B^{L} = \begin{pmatrix} 1 - \alpha & \beta \\ \alpha & 1 - \beta \end{pmatrix}, \qquad B^{R} = \begin{pmatrix} 1 - \gamma & \delta \\ \gamma & 1 - \delta \end{pmatrix}. \tag{10}$$

Next we consider the effect of virtual cell 0 on the left boundary block s_1u_2 . When cell 0 takes value $u_0 = 0$ with probability ζ , the upper left half of the matrix P acts on s_1u_2 . On the other hand, if $u_0 = 1$ with probability $1 - \zeta$, the bottom right half of P acts on s_1u_2 . Thus, the transition matrix on the left boundary cells s_1s_2 is

$$\tilde{P}^{L} = \zeta \begin{pmatrix} 1 & & & \\ & & 1 \\ & 1 & \end{pmatrix} + (1 - \zeta) \begin{pmatrix} & & 1 \\ & & & 1 \\ 1 & & \end{pmatrix}$$

$$= \begin{pmatrix} \zeta & & 1 - \zeta \\ & & & 1 \\ 1 - \zeta & & \zeta \\ & & 1 \end{pmatrix}. \tag{11}$$

By a similar argument, it is known that the effect of the right virtual cell is described by the following matrix:

$$\tilde{P}^{R} = \begin{pmatrix} \eta & 1 - \eta & & \\ 1 - \eta & \eta & & \\ & & & 1 \\ & & & 1 \end{pmatrix}. \tag{12}$$

The transition matrices at both boundaries are the compositions of P^L and B^L (left), P^R and B^R (right) as follows

$$P^{L} = \tilde{P}^{L}(\mathbf{1}_{2} \otimes B^{L}) = \begin{pmatrix} q_{1}^{L} & 1 - q_{2}^{L} \\ & \alpha & 1 - \beta \\ 1 - q_{1}^{L} & q_{2}^{L} \\ & 1 - \alpha & \beta \end{pmatrix}, \tag{13}$$

$$P^{R} = \tilde{P}^{R}(B^{R} \otimes \mathbf{1}_{2}) = \begin{pmatrix} q_{1}^{R} & 1 - q_{2}^{R} \\ 1 - q_{1}^{R} & q_{2}^{R} \\ & & \gamma & 1 - \delta \\ & & 1 - \gamma & \delta \end{pmatrix}.$$
 (14)

Here, $\mathbf{1}_2$ is a 2×2 unit matrix, and

$$q_1^L = \zeta + \alpha - 2\zeta\alpha, \qquad q_2^L = \zeta + \beta - 2\zeta\beta,$$
 (15)

$$q_1^R = \eta + \gamma - 2\eta\gamma, \qquad q_2^R = \eta + \delta - 2\eta\delta. \tag{16}$$

Since $0 \le \alpha, \beta, \gamma, \delta, \zeta, \eta \le 1$, these parameters also satisfy $0 \le q_1^L, q_2^L, q_1^R, q_2^R \le 1$.

The transition matrix U can be written as

$$U = U_o U_e, \tag{17}$$

$$U_e = P_{123}P_{345}P_{567}\cdots P_{n-3,n-2,n-1}P_{n-1,n}^R,$$
(18)

$$U_o = P_{12}^L P_{234} P_{456} P_{678} \cdots P_{n-2,n-1,n}, \tag{19}$$

where

$$P_{i-1,i,i+1} = \mathbf{1}_{2^{i-2}} \otimes P \otimes \mathbf{1}_{2^{n-i-1}}, \tag{20}$$

and

$$P_{12}^L = P_L \otimes \mathbf{1}_{2^{n-2}}, \qquad P_{n-1,n}^R = \mathbf{1}_{2^{n-2}} \otimes P^R.$$
 (21)

While U_e is the transition matrix corresponding to step (i), U_o is the transition matrix corresponding to step (ii). In this way the master equation for the system (7) is given. Note that all components of U are nonnegative and the sum of each column is 1. Namely, U is a stochastic matrix.

2.3. Nonequilibrium steady state

Although it is difficult to solve the master equation (7) in general, it is possible to solve for the steady state solution exactly. Here we describe the method of [9]. The steady state is the solution of the equation

$$\underline{p} = U\underline{p} \tag{22}$$

or

$$p_s = \sum_{s'} U_{ss'} p_{s'}. \tag{23}$$

Theses equations mean that \underline{p} is an eigenvector with eigenvalue 1 of the transition matrix U. We refer to (23) as a NESS equation, and to \underline{p} which satisfies (22) as a NESS vector. The existence and uniqueness of the NESS is guaranteed by the following theorem proved in [9].

Theorem 1. For all parameters $0 < \alpha, \beta, \gamma, \delta, \zeta, \eta < 1$, the transition matrix U is irreducible and aperiodic.

Here, *irreducible* means that there is a certain natural number $t_0 \in \mathbb{N}$ such that $(U^{t_0})_{s's} > 0$ for any s and s' and *aperiodic* means that for any s, the greatest common divisor of all t such that $(U^t)_{ss} > 0$ is 1. We do not prove this theorem here but according to the Perron-Frobenius's theorem, when U is irreducible and aperiodic, the maximum eigenvalue of a stochastic matrix is 1 and its eigenspace is one dimension [12]. Thus, the solution of the NESS equation (23) is unique.

We divide the master equation into

$$p_{s} = \sum_{s'} (U_{o})_{ss'} p'_{s'} \qquad p'_{s} = \sum_{s'} (U_{e})_{ss'} p_{s'},$$
 (24)

and assume the following patch state ansatz (PSA) that the solution can be written of the form:

$$p_{\mathbf{s}} = L_{s_1 s_2 s_3} X_{s_2 s_3 s_4 s_5} X_{s_4 s_5 s_6 s_7} \cdots X_{s_{n-4} s_{n-3} s_{n-2} s_{n-1}} R_{s_{n-2} s_{n-1} s_n}, \tag{25}$$

$$p'_{s} = L'_{s_1 s_2 s_3} X'_{s_2 s_3 s_4 s_5} X'_{s_4 s_5 s_6 s_7} \cdots X'_{s_{n-4} s_{n-3} s_{n-2} s_{n-1}} R'_{s_{n-2} s_{n-1} s_n}.$$
(26)

Here, X, X' are rank-4 tensors, and L, L', R, R' are rank-3 tensors of nonnegative components, which amount to $16 \times 2 + 8 \times 4 = 64$ unknown variables.

Normalisations: When the configuration is a vacuum state $\mathbf{s} = 0 \cdots 0$, (25) and (26) are

$$p_{0\cdots 0} = L_{000}(X_{0000})^{n/2-2} R_{000}, \qquad p'_{0\cdots 0} = L'_{000}(X'_{0000})^{n/2-2} R'_{000}.$$
 (27)

 U_e can change value of cell n and U_o value of cell 1, but the rest remains 0. Hence,

$$L_{000}(X_{0000})^{n/2-2}R_{000} = \sum_{s_n} (U_e)_{0\cdots 0s_n} L'_{000}(X'_{0000})^{n/2-2} R'_{00s_n}.$$
 (28)

Since this is true even if n change to n + 2, we can see by taking ratio of the two equations,

$$X_{0000} = X_{0000}' \tag{29}$$

Since the degree of freedom of constant multiplication is allowed for the partition function (total sum of probabilities), we can choose $X_{0000} = 1$.

Gauge symmetry: PSA (25) and (26) have gauge symmetry that makes the equation invariant. Let $f_{ss'}$, $f'_{ss'}$ be arbitrary 2-tensors. The NESS equation is then invariant under the following gauge transformation:

$$X_{ss'tt'} \mapsto f_{uu'} X_{ss'tt'} f_{tt'}^{-1},$$

$$L_{tss'} \mapsto L_{tss'} f_{ss'}^{-1},$$

$$R_{ss't} \mapsto f_{ss'} R_{ss't},$$
(30)

$$X'_{ss'tt'} \mapsto f'_{uu'} X'_{ss'tt'} f'^{-1}_{tt'},$$

$$L'_{tss'} \mapsto L'_{tss'} f'^{-1}_{ss'},$$

$$R'_{ss't} \mapsto f'_{ss'} R'_{ss't}.$$

$$(31)$$

So if we fix gauge to

$$f_{ss'} = (L_{000}, X_{0001}, X_{0010}, X_{0011}), (32)$$

$$f'_{ss'} = (R'_{000}, X'_{0001}, X'_{0010}, X'_{0011}), (33)$$

we can transform the PSA components into

$$L_{000}, R'_{000}, X_{00ss'}, X'_{00ss'} \mapsto 1.$$
 (34)

Note that under this gauge transformation, the diagonal components are invariant, $X_{ss's'} \mapsto f_{ss'}X_{ss'ss'}f_{ss'}^{-1} = X_{ss'ss'}$.

Thus, the number of unknown variables in the equations is reduced to 64-2-2-6=54. If we successfully determine the 54 unknowns and get a solution for the equations, PSA gives the unique solution.

Matrix representation of the tensors: Here we express the tensors in PSA in matrix form. $X_{ss'tt'}$, $X'_{ss'tt'}$ can be represented by 4×4 matrices whose rows are labeled by ss' (in order of 00, 01, 10, 11) and whose columns labeled by tt'. Then, let unknown components of the matrices be

$$X = \begin{pmatrix} 1 & 1 & 1 & 1 \\ y_1 & y_2 & y_3 & y_4 \\ y_5 & y_6 & y_7 & y_8 \\ y_9 & y_{10} & y_{11} & y_{12} \end{pmatrix}, \tag{35}$$

$$X' = \begin{pmatrix} 1 & 1 & 1 & 1 \\ y'_1 & y'_2 & y'_3 & y'_4 \\ y'_5 & y'_6 & y'_7 & y'_8 \\ y'_9 & y'_{10} & y'_{11} & y'_{12} \end{pmatrix}. \tag{36}$$

Similarly $L_{tss'}$, $L'_{tss'}$ and $R_{ss't}$, $R'_{ss't}$ can be represented by using 2×4 , 4×2 matrices respectively,

$$L = \begin{pmatrix} 1 & l_2 & l_3 & l_4 \\ l_5 & l_6 & l_7 & l_8 \end{pmatrix}, \qquad L' = \begin{pmatrix} l'_1 & l'_2 & l'_3 & l'_4 \\ l'_5 & l'_6 & l'_7 & l'_8 \end{pmatrix}, \tag{37}$$

$$R = \begin{pmatrix} r_1 & r_2 \\ r_3 & r_4 \\ r_5 & r_6 \\ r_7 & r_8 \end{pmatrix}, \qquad R' = \begin{pmatrix} 1 & r_2' \\ r_3' & r_4' \\ r_5' & r_6' \\ r_7' & r_8' \end{pmatrix}.$$
(38)

Reduced NESS equations: The 54 unknowns can be determined by examining specific components of the NESS vectors. First, we focus on the following components: (I) all indices except s_1 , s_2 , s_3 are 0, (II) all indices except s_{n-2} , s_{n-1} , s_n are 0, (III) all indices except s_{2k+2} , s_{2k+3} , s_{2k+4} , s_{2k+5} , (0 < k < n/2 - 3) are 0. In each case, calculating the NESS equation (23) directly, we obtain

$$L'_{s_1 s_2 s_3} X'_{s_2 s_3 00} = \sum_{t_n} (P^R)_{000t_n} R_{00t_n} L_{s_1 \chi(s_1 s_2 s_3) s_3} X_{\chi(s_1 s_2 s_3) s_3 s_3 0} X_{s_3 000}, \quad (39)$$

$$L_{s_1 s_2 s_3} X_{s_2 s_3 00} R_{000} = \sum_{t_1} (P^L)_{s_1 s_2 t_1 s_2} L'_{t_1 s_2 \chi(s_2 s_3 0)} X'_{s_2 \chi(s_2 s_3 0) 00}, \tag{40}$$

$$L'_{000}R'_{s_{n-2}s_{n-1}s_n} = \sum_{t_n} (P^R)_{s_{n-1}s_ns_{n-1}t_n},$$
(41)

$$R_{s_{n-2}s_{n-1}s_n} = \sum_{t_1} (P^L)_{00t_10} L'_{t_100} X'_{0s_{n-2}s_{n-2}\chi(s_{n-2}s_{n-1}s_n)} R'_{s_{n-2}\chi(s_{n-2}s_{n-1}s_n)s_n}, (42)$$

$$L'_{000}X'_{s_2s_3s_4s_5}X'_{s_4s_500} = \sum_{t_n} (P^R)_{000t_n} R_{00t_n} X_{\chi(0s_2s_3)s_3\chi(s_3s_4s_5)s_5} X_{\chi(s_3s_4s_5)s_5s_50} X_{s_5000}, \tag{43}$$

$$X_{s_2s_3s_4s_5}X_{s_4s_500}R_{000} = \sum_{t_1} (P^L)_{00t_10}L'_{t_100}X_{0s_2s_2\chi(s_2s_3s_4)}X_{s_2\chi(s_2s_3s_4)s_4\chi(s_4s_50)}X_{s_4\chi(s_4s_50)00}.$$
(44)

In (43) and (44), we have replaced s_{2k+2} , s_{2k+3} , s_{2k+4} , s_{2k+5} by $s_2s_3s_4s_5$ for simplicity of presentation. Solving these equations, we have

$$X = \begin{pmatrix} 1 & 1 & 1 & 1 \\ y_1 & y_2 & y_3 & y_4 \\ y_1 & y_4/y_3 & y_2 & y_4/y_3 \\ y_1/y_4 & 1/y_3 & 1 & y_2 \end{pmatrix},$$

$$X' = \begin{pmatrix} 1 & 1 & 1 & 1 \\ y_1 & y_2 & 1/y_4 & 1/y_3 \\ y_1 & y_4/y_3 & y_2 & y_4/y_3 \\ y_1y_3 & y_4 & 1 & y_2' \end{pmatrix},$$

$$L = \begin{pmatrix} 1 & l_2 & l_3 & l_4 \\ l_5 & l_6 & l_7 & l_8 \end{pmatrix}, \qquad L' = \begin{pmatrix} l'_1 & l'_1l_4 & l'_1l_3 & l'_1l_2 \\ l'_1l_7y_1 & l_1l'_8 & l'_1l_5/y_1 & l'_1l_6 \end{pmatrix},$$

$$R = \begin{pmatrix} r_1 & r_2 \\ r_3 & r_4 \\ r_5 & r_6 \\ r_7 & r_8 \end{pmatrix}, \qquad R' = \begin{pmatrix} 1 & r_4/r_1 \\ r_3/r_1 & r_2/r_1 \\ y_1y_3r_7/r_1 & y_1y_3r_8/r_1 \\ r_5/(y_3r_1) & r_6/(y_3r_1) \end{pmatrix}.$$

There are still remained 4 + 7 + 1 + 8 = 20 undetermined variables in PSA, which are related by

$$l'_{1} = q_{1}^{R}r_{1} + (1 - q_{2}^{R})r_{2},$$

$$l'_{1}r_{2} = r_{1}[(1 - \gamma)r_{7} + \delta r_{8}],$$

$$l'_{1}r_{3} = r_{1}[\gamma r_{7} + (1 - \delta)r_{8}],$$

$$l'_{1}r_{4} = r_{1}[(1 - q_{1}^{R})r_{1} + q_{2}^{R}r_{2}],$$

$$l'_{1}r_{5} = r_{1}/y_{3} \cdot [\gamma r_{3} + (1 - \delta)r_{4}],$$

$$l'_{1}r_{6} = r_{1}/y_{3} \cdot [(1 - \gamma)r_{3} + \delta r_{4}],$$

$$l'_{1}r_{7} = r_{1}/y_{4} \cdot [q_{1}^{R}r_{5} + (1 - q_{2}^{R})r_{6}],$$

$$l'_{1}r_{8} = r_{1}/y_{4} \cdot [(1 - q_{1}^{R})r_{5} + q_{2}^{R}r_{6}],$$

$$r_{1} = l'_{1}[q_{1}^{L} + (1 - q_{2}^{L})l_{7}y_{1}],$$

$$r_{1}l_{2} = l'_{1}[q_{1}^{L}l_{4} + (1 - q_{2}^{L})l_{8}],$$

$$r_{1}l_{3} = l'_{1}y_{3}[\alpha l_{2} + (1 - \beta)l_{6}],$$

$$r_{1}l_{4} = l'_{1}y_{4}/y_{1} \cdot [\alpha l_{3}y_{1} + (1 - \beta)l_{5}],$$

$$r_{1}l_{5} = l'_{1}[1 - q_{1}^{L} + q_{2}^{L}l_{7}y_{1}],$$

$$r_{1}l_{6} = l'_{1}[(1 - q_{1}^{L})l_{4} + q_{2}^{L}l_{8}],$$

$$r_{1}l_{7} = l'_{1}y_{3}[(1 - \alpha)l_{2} + \beta l_{6}],$$

$$r_{1}l_{8} = l'_{1}y_{4}/y_{1} \cdot [(1 - \alpha)l_{3}y_{1} + \beta l_{5}].$$
(46)

However, since all unknowns cannot be determined by these equations alone, other component equations are required.

Next, we focus on the following components: (IV) all indices except $s_{2k+2}, s_{2k+3}, s_{2k+4}, s_{2k+5}, (0 < k < n/2-3)$ are 1, (V) all indices except $s_2, s_3, s_4, s_5, (k = 0)$ are 0, (VI) all indices except $s_{n-4}, s_{n-3}, s_{n-2}, s_{n-1}, (k = n/2 - 3)$ are 0. From these components, we obtain the following equations,

$$y_{2} = y_{1},$$

$$y_{4} = y_{1}y_{3},$$

$$l'_{1}y_{1} = q_{1}^{R}r_{5} + (1 - q_{2}^{R})r_{6},$$

$$l'_{1}r'_{5} = y_{1}[q_{1}^{R}r_{1} + (1 - q_{2}^{R})r_{2}],$$

$$r_{1} = l'_{1}[q_{1}^{L}l_{4} + (1 - q_{2}^{L})l_{8}],$$

$$r_{1}l_{2} = l'_{1}[q_{1}^{L} + (1 - q_{2}^{L})^{L}l_{7}y_{1}].$$

$$(47)$$

Thus, we can represent y_2 and y_4 using y_1 and y_3 , and moreover find relations $l_2 = 1$ and $r_7 = r_1/y_3$. The remaining unknowns are $y_1, y_3, l_3, \ldots, l_8, r_1, \ldots, r_8$, and l'_1 . Because all

components of R and L' include l'_1 as a factor, and the PSA also does, we can set $l'_1 = 1$ using the freedom of multiplying a constant to the eigenvector.

Exact solutions of the reduced NESS equations: It is still difficult to solve (45) and (46). However, there are cases where a special relation holds between parameters, the equations become simpler and an exact solution is obtained. In the previous study [9], the exact solution for $\zeta = \eta = 1/2$ is given. This case is called Bernoulli driving in [11]. Here we will show that an exact solution is obtained for arbitrary ζ and η if the conditions

$$\alpha = 1 - \beta, \quad \gamma = 1 - \delta \tag{48}$$

are satisfied. They mean that when updating the boundary cells, the probability of $s_1 = 1$ is α and that of $s_n = 1$ is γ irrespective of the previous values of s_1 and s_n . Both of the two cases are united into $q_1^L = 1 - q_2^L$ and $q_1^R = 1 - q_2^R$, and the linear combinations of r_i and l_i in the right hand side of (45) and (46) become simple. In the latter case, P^L and P^R in (13) and (14) are

$$P^{L} = \begin{pmatrix} q_{1}^{L} & q_{1}^{L} & \\ & \alpha & & \alpha \\ 1 - q_{1}^{L} & 1 - q_{1}^{L} & \\ & 1 - \alpha & 1 - \alpha \end{pmatrix}, \tag{49}$$

$$P^{R} = \begin{pmatrix} q_{1}^{R} & q_{1}^{R} & & & \\ 1 - q_{1}^{R} & 1 - q_{1}^{R} & & & \\ & & \gamma & \gamma & \\ & & 1 - \gamma & 1 - \gamma \end{pmatrix}.$$
 (50)

These boundary stochastic matrices actually operate on the states of cells 1 and 2 without referring to the virtual cells 0 and n+1. For example, the above P_L means that cell 1 at next time takes 0 with probability q_1^L if $s_2 = 0$ and with probability α if $s_2 = 1$. Thus, these are essentially equivalent to the conditional driving boundary conditions in [11]: q_1^L and α in (49) correspond to α and β in (13) of [11], respectively, and q_1^R and γ in (50) to γ and δ in [11]. The only difference is that q_1^L and q_1^R depend on α and γ in our case, while all the parameters in [11] are independent of each other. However, we do not utilize the dependence in the following treatment, which can thus also be applied to the conditional boundary driving case.

When
$$q_1^L = 1 - q_2^L$$
 and $q_1^R = 1 - q_2^R$, the NESS equations are simplified as
$$1 = q_1^R(r_1 + r_2),$$

$$r_2 = r_1(1 - \gamma)(r_7 + r_8),$$

$$r_3 = r_1\gamma(r_7 + r_8),$$

$$r_4 = r_1(1 - q_1^R)(r_1 + r_2),$$

$$r_5 = r_1/y_3 \cdot \gamma(r_3 + r_4),$$

$$r_6 = r_1/y_3 \cdot (1 - \gamma)(r_3 + r_4),$$

$$r_{7} = r_{1}/(y_{1}y_{3}) \cdot q_{1}^{R}(r_{5} + r_{6}),$$

$$r_{8} = r_{1}/(y_{1}y_{3}) \cdot (1 - q_{1}^{R})(r_{5} + r_{6}),$$

$$r_{1} = q_{1}^{L}(1 + l_{7}y_{1}),$$

$$r_{1} = q_{1}^{L}(l_{4} + l_{8}),$$

$$r_{1}l_{3} = y_{3}\alpha(1 + l_{6}),$$

$$r_{1}l_{4} = y_{3}\alpha(l_{3}y_{1} + l_{5}),$$

$$r_{1}l_{5} = (1 - q_{1}^{L})(1 + l_{7}y_{1}),$$

$$r_{1}l_{6} = (1 - q_{1}^{L})(l_{4} + l_{8}),$$

$$r_{1}l_{7} = y_{3}(1 - \alpha)(1 + l_{6}),$$

$$r_{1}l_{8} = y_{3}(1 - \alpha)(l_{3}y_{1} + l_{5}),$$

$$(52)$$

$$r_{7} = r_{1}/y_{3}.$$

Then we arrive at the same form of transfer matrices as (43) in [9]

$$X = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \xi \omega & \xi \omega & \xi^{-1} & \omega \\ \xi \omega & \xi \omega & \xi \omega & \xi \omega \\ \xi & \xi & 1 & \xi \omega \end{pmatrix}, \quad X' = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \xi \omega & \xi \omega & \omega^{-1} & \xi \\ \xi \omega & \xi \omega & \xi \omega & \xi \omega \\ \omega & \omega & 1 & \xi \omega \end{pmatrix}$$
(54)

where

$$\xi := \frac{1}{y_3} = \frac{(1 - \gamma)\alpha + (1 - \alpha)q_1^R}{[(1 - \alpha)\gamma + (1 - \gamma)q_1^L]^2} \left(\alpha + (1 - \alpha)q_1^R - q_1^L q_1^R\right),\tag{55}$$

and

$$\omega := y_1 y_3 = \frac{(1 - \alpha)\gamma + (1 - \gamma)q_1^L}{[(1 - \gamma)\alpha + (1 - \alpha)q_1^R]^2} \Big(\gamma + (1 - \gamma)q_1^L - q_1^L q_1^R\Big), \tag{56}$$

Matrices L, L', R, and R' are written with the following quantities.

$$r_{1} = \frac{(1-\alpha)\gamma + (1-\gamma)q_{1}^{L}}{(1-\gamma)\alpha + (1-\alpha)q_{1}^{R}},$$

$$r_{2} = \frac{1-\gamma}{q_{1}^{R}[(1-\gamma)\alpha + (1-\alpha)q_{1}^{R}]} \left(\alpha + (1-\alpha)q_{1}^{R} - q_{1}^{L}q_{1}^{R}\right),$$

$$r_{3} = \frac{\gamma}{q_{1}^{R}[(1-\gamma)\alpha + (1-\alpha)q_{1}^{R}]} \left(\alpha + (1-\alpha)q_{1}^{R} - q_{1}^{L}q_{1}^{R}\right),$$

$$r_{4} = \left(\frac{1}{q_{1}^{R}} - 1\right) \frac{(1-\alpha)\gamma + (1-\gamma)q_{1}^{L}}{(1-\gamma)\alpha + (1-\alpha)q_{1}^{R}},$$

$$r_{5} = \frac{\gamma}{q_{1}^{R}} \frac{[\alpha + (1-\alpha)q_{1}^{R} - q_{1}^{L}q_{1}^{R}][\gamma + (1-\gamma)q_{1}^{L} - q_{1}^{L}q_{1}^{R}]}{[(1-\alpha)\gamma + (1-\gamma)q_{1}^{L}][(1-\gamma)\alpha + (1-\alpha)q_{1}^{R}]},$$

$$r_{6} = \frac{1-\gamma}{q_{1}^{R}} \frac{[\alpha + (1-\alpha)q_{1}^{R} - q_{1}^{L}q_{1}^{R}][\gamma + (1-\gamma)q_{1}^{L} - q_{1}^{L}q_{1}^{R}]}{[(1-\alpha)\gamma + (1-\gamma)q_{1}^{L}][(1-\gamma)\alpha + (1-\alpha)q_{1}^{R}]},$$

$$r_{7} = \frac{\alpha + (1-\alpha)q_{1}^{R} - q_{1}^{L}q_{1}^{R}}{(1-\alpha)\gamma + (1-\gamma)q_{1}^{L}},$$

$$r_{8} = \left(\frac{1}{q_{1}^{R}} - 1\right) \frac{\alpha + (1-\alpha)q_{1}^{R} - q_{1}^{L}q_{1}^{R}}{(1-\alpha)\gamma + (1-\gamma)q_{1}^{L}},$$
(57)

$$l_{3} = \frac{\alpha}{q_{1}^{L}} \frac{(1-\alpha)\gamma + (1-\gamma)q_{1}^{L}}{\alpha + (1-\alpha)q_{1}^{R} - q_{1}^{L}q_{1}^{R}},$$

$$l_{4} = \frac{\alpha}{q_{1}^{L}} \frac{(1-\alpha)\gamma + (1-\gamma)q_{1}^{L}}{(1-\gamma)\alpha + (1-\alpha)q_{1}^{R}},$$

$$l_{5} = l_{6} = \frac{1}{q_{1}^{L}} - 1,$$

$$l_{7} = \frac{1-\alpha}{q_{1}^{L}} \frac{(1-\alpha)\gamma + (1-\gamma)q_{1}^{L}}{\alpha + (1-\alpha)q_{1}^{R} - q_{1}^{L}q_{1}^{R}},$$

$$l_{8} = \frac{1-\alpha}{q_{1}^{L}} \frac{(1-\alpha)\gamma + (1-\gamma)q_{1}^{L}}{(1-\gamma)\alpha + (1-\alpha)q_{1}^{R}}.$$
(58)

2.4. Physical quantities in the NESS

Partition function: Since the NESS vectors p_s , p'_s are obtained, we can calculate the expectation value of physical quantities with these vectors. Partition functions of the system are

$$Z_n := \sum_{\mathbf{s}} p_{\mathbf{s}}, \qquad Z'_n = \sum_{\mathbf{s}} p'_{\mathbf{s}}. \tag{59}$$

Substituting the PSA (25) and (26) gives the following matrix product forms:

$$Z_n = \mathbf{l} X^{n/2-2} \mathbf{r}, \qquad Z'_n = \mathbf{l}' X'^{n/2-2} \mathbf{r}'. \tag{60}$$

Here we introduced a four component vectors

$$\mathbf{l} := (L_{0ss'} + L_{1ss'}), \qquad \mathbf{l}' := (L'_{0ss'} + L'_{1ss'}),
\mathbf{r} := (R_{ss'0} + R_{ss'1}), \qquad \mathbf{r}' := (R'_{ss'0} + R'_{ss'1}). \tag{61}$$

In the case of exact solution (55)-(58),

$$lX = \tau_1 l Xr = \tau_1 r,$$

$$l'X' = \tau_1 l' X'r' = \tau_1 r',$$
(62)

$$\tau_1 = \frac{[1 - (1 - 2\alpha)(1 - 2\gamma)(1 - \zeta)(1 - \eta)]^2}{[(1 - \gamma)\alpha + (1 - \alpha)q_1^R][(1 - \alpha)\gamma + (1 - \gamma)q_1^L]}$$
(63)

are satisfied. That is, \boldsymbol{l} and \boldsymbol{r} are eigenvectors of X belonging to the eigenvalue τ_1 . By using this fact repeatedly,

$$Z_n = \tau_1^{n/2-2} \boldsymbol{l} \cdot \boldsymbol{r}, \qquad Z_n' = \tau_1^{n/2-2} \boldsymbol{l}' \cdot \boldsymbol{r}'. \tag{64}$$

From direct calculation, we obtain

$$\mathbf{l} \cdot \mathbf{r} = \mathbf{l}' \cdot \mathbf{r}' = \frac{\alpha \gamma - 2\alpha - 2\gamma - 2(1 - \alpha)q_1^R - 2(1 - \gamma)q_1^L + 3q_1^L q_1^R}{q_1^L q_1^R [(1 - \gamma)\alpha - (1 - \alpha)q_1^R]}.$$
 (65)

Hence, $Z_n = Z'_n$. In the following, we calculate expectation values with Z_n .

Density: We define the density of 1 at cell i as

$$\rho_i := \frac{1}{Z_n} \sum_{\mathbf{s}} s_i p_{\mathbf{s}} \tag{66}$$

First consider the case $i=2k, (k=1, \dots, n/2-1)$. Substituting the PSA (25), it becomes

$$\rho_{2k} = \frac{1}{Z_n} \sum_{s_{2k}, s_{2k+1}} (\boldsymbol{l} X^{k-1})_{s_{2k}, s_{2k+1}} s_{2k} (X^{n/2-k-1} \boldsymbol{r})_{s_{2k}, s_{2k+1}}.$$

Because X is replaced with τ_1 by acting on \boldsymbol{l} or \boldsymbol{r} as in (62), we have

$$\rho_{2k} = \frac{\tau_1^{n/2-2}}{Z_n} \sum_{s_{2k}, s_{2k+1}} l_{s_{2k}s_{2k+1}} s_{2k} r_{s_{2k}s_{2k+1}}$$

Substituting the exact solution, we arrive at

$$\rho_{2k} = \frac{-\alpha - \gamma - (1 - \alpha)q_1^R - (1 - \gamma)q_1^L + 2q_1^L q_1^R}{\alpha \gamma - 2\alpha - 2\gamma - 2(1 - \alpha)q_1^R - 2(1 - \gamma)q_1^L + 3q_1^L q_1^R}.$$
(67)

Similarly, we can derive that $\rho_{2k+1} = \rho_{2k}$ for $k = 1, \dots, n/2 - 1$. Thus the density of 1 is uniform in $2 \le i \le n - 1$ and its value is denoted by ρ in the following.

Finally, unlike bulk, the densities at boundary i=1,n are calculated by the formulas

$$\rho_{1} = \frac{\tau_{1}^{n/2-2}}{Z_{n}} \sum_{s_{1}, s_{2}, s_{3}} L_{s_{1}s_{2}s_{3}} s_{1} r_{s_{2}s_{3}},$$

$$\rho_{n} = \frac{\tau_{1}^{n/2-2}}{Z_{n}} \sum_{s_{n-2}, s_{n-1}, s_{n}} l_{s_{n-2}s_{n-1}} s_{n} R_{s_{n-2}s_{n-1}s_{n}}$$
(68)

which produces lengthy equations we do not show here. Those values are different from the bulk density.

Let us examine the range of values for the bulk density. For the emission limit α , $\gamma \to 1$, the density takes the maximum value 2/3 regardless of ζ , η . On the other hand, for the absorption limit α , $\gamma \to 0$, it become

$$\rho = \frac{2-x}{3-2x}, \qquad x = \frac{1}{\zeta} + \frac{1}{\eta}.$$

In the range of $0 < \zeta$, $\eta < 1$, x is in $2 < x < \infty$ and the density is in $0 < \rho < 1/2$. Thus, the density can take a value in the range $0 < \rho < 2/3$. The fact that the maximum value of the density is 2/3 instead of 1 is directly understood from the rule (5). The rule allows $s_{2k}^t = s_{2k}^{t+1} = 1$ only in the case $s_{2k-1}^t = s_{2k+1}^t = 0$, which inevitably leads to $s_{2k-1}^{t+1} = s_{2k+1}^{t+1} = 1$ because $\chi(*,0,1) = \chi(1,0,*) = 1$. Then, $s_{2k}^{t+2} = \chi(s_{2k-1}^{t+1}, s_{2k}^{t+1}, s_{2k+1}^{t+1}) = \chi(1,1,1) = 0$. Thus any cell cannot have 1 three times in a row. Thus the density of 1 is bounded above by 2/3. It is interesting that our solution covers all possible values of the density, whereas the bulk steady-state density can only take values in interval (2/5, 2/3) for the solution in [9]

Current: As in [10, 9], the particle current is defined as the expectation value of the density of right-movers minus that of left-movers $J = J_R - J_L$, where

$$J_R := \frac{1}{Z_n} \sum_{s} s_{2k} s_{2k+1} p_s,$$

$$J_L := \frac{1}{Z_n} \sum_{s} s_{2k+1} s_{2k+2} p_s.$$
(69)

Substituting the PSA(25) and using (62), J_R is obtained as

$$J_{R} = \frac{\tau_{1}^{n/2-2}}{Z_{n}} \sum_{s_{2k}, s_{2k+1}} l_{s_{2k}s_{2k+1}} s_{2k} s_{2k+1} r_{s_{2k}s_{2k+1}}$$

$$= \frac{-\alpha - (1-\alpha)q_{1}^{R} + q_{1}^{L} q_{1}^{R}}{\alpha \gamma - 2\alpha - 2\gamma - 2(1-\alpha)q_{1}^{R} - 2(1-\gamma)q_{1}^{L} + 3q_{1}^{L} q_{1}^{R}}.$$
(70)

Quite similarly, J_L is obtained as

$$J_L = \frac{-\gamma - (1 - \gamma)q_1^R + q_1^L q_1^R}{\alpha\gamma - 2\alpha - 2\gamma - 2(1 - \alpha)q_1^R - 2(1 - \gamma)q_1^L + 3q_1^L q_1^R}.$$
 (71)

Thus, we arrive at

$$J = \frac{(\gamma - \alpha)(2 - \alpha - \gamma) + \eta(1 - \gamma)(1 - 2\gamma) - \zeta(1 - \alpha)(1 - 2\alpha)}{\alpha\gamma - 2\alpha - 2\gamma - 2(1 - \alpha)q_1^R - 2(1 - \gamma)q_1^L + 3q_1^L q_1^R}.$$
 (72)

In the case where $\eta = \zeta$ and difference between α and γ is small, the current is approximately proportional to $\gamma - \alpha$.

We notice another interesting relation

$$J_L + J_R = \rho. (73)$$

This is also explained in the same manner as for the maximum value of the bulk density. Assume $(s_{2k-1}^t, s_{2k}^t, s_{2k+1}^t) = (0, 1, 0)$. Then, $s_{2k}^{t+1} = \chi(s_{2k-1}^t, s_{2k}^t, s_{2k+1}^t) = 1$, and because $\chi(*,0,1) = \chi(1,0,*) = 1$, $s_{2k-1}^{t+1} = \chi(s_{2k-2}^{t+1}, s_{2k-1}^t, s_{2k-1}^{t+1}) = 1$ and $s_{2k+1}^{t+1} = \chi(s_{2k}^{t+1}, s_{2k+1}^t, s_{2k+2}^{t+1}) = 1$, namely we obtain $(s_{2k-1}^{t+1}, s_{2k}^{t+1}, s_{2k+1}^{t+1}) = (1, 1, 1)$. The time-reversal symmetry of the rule (6) ensures that the inverse is true; if $(s_{2k-1}^{t+1}, s_{2k}^{t+1}, s_{2k+1}^{t+1}) = (1, 1, 1)$, we have $(s_{2k-1}^t, s_{2k}^t, s_{2k+1}^t) = (0, 1, 0)$. Similarly, we can derive that $(s_{2k}^{t+1}, s_{2k+1}^{t+1}, s_{2k+2}^{t+1}) = (0, 1, 0)$ if and only if $(s_{2k}^t, s_{2k+1}^t, s_{2k+2}^t) = (1, 1, 1)$. These properties leads to that the marginal distribution $p(s_{i-1}, s_i, s_{i+1})$ in a stationary state must satisfy p(0, 1, 0) = p(1, 1, 1) for $2 \le i \le N - 2$. Using the marginal distribution, we can write $J_R = p(1, 1, 0) + p(1, 1, 1)$, $J_L = p(0, 1, 1) + p(1, 1, 1)$ and $\rho_i = p(0, 1, 0) + p(1, 1, 0) + p(0, 1, 1) + p(1, 1, 1)$. Thus the relation (73) is derived from p(0, 1, 0) = p(1, 1, 1). This relation must be satisfied in any stationary states.

3. Temperature driven RCA 54

3.1. The relation between RCA54 and ERCA 250R

Before introducing the boundary condition, we discuss the relation between Bobenko's RCA54 and ERCA 250R. As mentioned in Introduction, ERCA 250R is given by (1)

with f(0,0,0) = f(0,1,0) = 0 and f(x,y,z) = 1 for all other combinations of (x,y,z). It is also represented as

$$x_i^{\tau+1} = x_{i-1}^{\tau} \oplus x_{i+1}^{\tau} \oplus x_{i-1}^{\tau} x_{i+1}^{\tau} \oplus x_i^{\tau-1}, \tag{74}$$

where we have changed t to τ . It should be noted that the right hand side of this equation does not depend on x_i^{τ} . This property leads to the fact that spatiotemporal evolution $\{x_i^{\tau}\}$ with $i+\tau=$ even and that with $i+\tau=$ odd are independent of each other. In the former set, if we write $s_{2k}^t=x_{2k}^{2t}$ and $s_{2k+1}^t=x_{2k+1}^{2t+1}$, s_{2k}^{t+1} is determined by (3) and s_{2k+1}^{t+1} is determined by (4). The set $\{x_i^{\tau}\}$ with $i+\tau=$ odd is similarly regarded as the evolution of RCA54. That is, ERCA rule 250R is decomposed into two independent RCA54. It is illustrated in Figure 7.

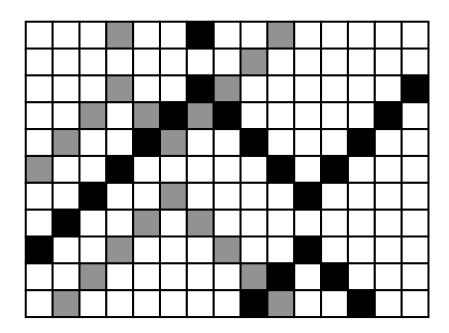


Figure 7. Time evolution of s_i according to ERCA rule 250R. Each column represents the configuration at each time and the time flows downward. White represents the value 0, black and gray represent the value 1. It can be seen that blacks collide and shift by two steps, and grays behave similarly, but black and gray pass through.

3.2. Heat-bath boundary conditions

We introduce here a heat-bath boundary condition to RCA54 in the same manner as is done in [7] for ERCA. To do so, we have to identify an additive conserved quantity for RCA54. It is shown in [8] that ERCA rule 250R has several such conserved quantities. We adapt the result to RCA54 and obtain that

$$E_i^t := (-1)^{i+1} |s_i^t - s_{i+1}^t| = \begin{cases} (-1)^{i+1} & s_i \neq s_{i+1} \\ 0 & s_i = s_{i+1} \end{cases}$$
 (75)

is a conserved density, which is interpreted as energy in the following. Note that the energy is not carried by particles but lies between cells. The conservation can be verified directly from the equality of χ

$$|x - y| - |y - z| = |\chi(x, y, z) - z| - |x - \chi(x, y, z)|, \tag{76}$$

which means that the sum of energy is conserved for each diamond-shaped plaquette. The conservation law is also written in the form of the equation of continuity

$$E_i^{t+1} - E_i^t = -\left(S_{i+1}^t - S_i^t\right). \tag{77}$$

with energy current

$$S_i^t := 1 - s_i^t - s_i^{t+1}. (78)$$

Though the constant in the right-hand side can be chosen arbitrarily, we set it to unity for later convenience.

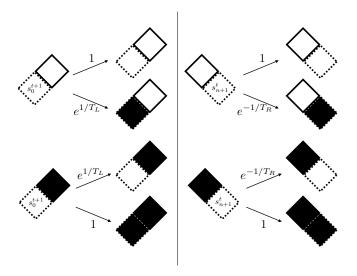


Figure 8. Boundary conditions assumed that thermal bath is in contact. The weights of the values taken by the virtual cells are determined according to the values of the cells 1, n.

Next, we devise the heat-bath boundary condition by assigning Gibbs weights for the values of the virtual cells 0 and n + 1:

$$P_{s_0} = \frac{1}{N_L} e^{-E_0/T_L}, \qquad P_{s_{n+1}} = \frac{1}{N_R} e^{-E_n/T_R}.$$
 (79)

Here, T_L and T_R mean the "temperature" of the thermal baths in contact at the left and right boundaries, respectively, and $N_L = 1 + e^{1/T_L}$ and $N_R = 1 + e^{-1/T_R}$ are normalization factors. Note that because the energy is bounded, T_L and T_R can take negative values. In this boundary condition, \tilde{P}^L in (11) and \tilde{P}^R in (12) are replaced by

$$\tilde{P}^{L} = \begin{pmatrix} 1/N_{L} & 1/N_{L} & \\ & & 1\\ e^{1/T_{L}}/N_{L} & e^{1/T_{L}}/N_{L} & \\ & 1 & \end{pmatrix},$$

$$\tilde{P}^{R} = \begin{pmatrix} 1/N_{R} & 1/N_{R} & \\ e^{-1/T_{R}}/N_{R} & e^{-1/T_{R}}/N_{R} & \\ & & 1 \\ & & 1 \end{pmatrix}.$$

$$(80)$$

With (11), the boundary transition matrices are determined as follows:

Since the bulk transition matrix remains unchanged, we only have to replace the parameters in the previous section as follows

$$\begin{aligned} q_1^L, \ 1 - q_2^L &\to 1/N_L, & 1 - q_1^L, \ q_2^L &\to e^{1/T_L}/N_L, \\ q_1^R, \ 1 - q_2^R &\to 1/N_R, & 1 - q_1^R, \ q_2^R &\to e^{-1/T_R}/N_R. \end{aligned}$$

The reduced NESS equations are immediately obtained:

$$1 = (r_{1} + r_{2})/N_{R},$$

$$r_{2} = r_{1}[(1 - \gamma)r_{7} + \delta r_{8}],$$

$$r_{3} = r_{1}[\gamma r_{7} + (1 - \delta)r_{8}],$$

$$r_{4} = r_{1}(r_{1} + r_{2})e^{-1/T_{R}}/N_{R},$$

$$r_{5} = r_{1}[\gamma r_{3} + (1 - \delta)r_{4}]/y_{3},$$

$$r_{6} = r_{1}[(1 - \gamma)r_{3} + \delta r_{4}]/y_{3},$$

$$r_{7} = r_{1}(r_{5} + r_{6})/(y_{1}y_{3}N_{R}),$$

$$r_{8} = r_{1}(r_{5} + r_{6})e^{-1/T_{R}}/(y_{1}y_{3}N_{R}),$$

$$r_{1} = (1 + l_{7}y_{1})/N_{L},$$

$$r_{1} = (l_{4} + l_{8})/N_{L},$$

$$r_{1}l_{3} = y_{3}[\alpha + (1 - \beta)l_{6}],$$

$$r_{1}l_{4} = y_{3}[\alpha l_{3}y_{1} + (1 - \beta)l_{5}],$$

$$r_{1}l_{5} = (1 + l_{7}y_{1})e^{1/T_{L}}/N_{L},$$

$$r_{1}l_{6} = (l_{4} + l_{8})e^{1/T_{L}}/N_{L},$$

$$r_{1}l_{7} = y_{3}[1 - \alpha + \beta l_{6}],$$

$$r_{1}l_{8} = y_{3}[(1 - \alpha)l_{3}y_{1} + \beta l_{5}],$$
(83)
$$r_{7} = r_{1}/y_{3}.$$

These new reduced NESS equations (82)-(84) are solved exactly. Again, we obtain the transfer matrices X and X' of the form (54) with

$$\xi := \frac{1}{y_3} = \frac{1 - \lambda \mu + (1 - \mu)e^{1/T_L}}{[1 - \lambda \mu + (1 - \lambda)e^{-1/T_R}]^2} \Big(\lambda e^{-1/T_R} + e^{1/T_L}(1 + e^{-1/T_R})\Big), \quad (85)$$

$$\omega := y_1 y_3 = \frac{1 - \lambda \mu + (1 - \lambda)e^{-1/T_R}}{[1 - \lambda \mu + (1 - \mu)e^{1/T_L}]^2} \Big(\mu e^{1/T_L} + e^{-1/T_R} (1 + e^{1/T_L}) \Big), \quad (86)$$

and the matrices L and R with parameters

$$r_{1} = \frac{1 - \lambda \mu + (1 - \lambda)e^{-1/T_{R}}}{1 - \lambda \mu + (1 - \mu)e^{1/T_{L}}},$$

$$r_{2} = (1 - \mu) \frac{\lambda e^{-1/T_{R}} + e^{1/T_{L}}(1 + e^{-1/T_{R}})}{1 - \lambda \mu + (1 - \mu)e^{1/T_{L}}},$$

$$r_{3} = r_{1}^{2} \xi(e^{-1/T_{R}} + \mu),$$

$$r_{4} = r_{1}e^{-1/T_{R}},$$

$$r_{5} = r_{1} \xi[\gamma r_{3} + (1 - \delta)r_{4}],$$

$$r_{6} = r_{1} \xi[(1 - \gamma)r_{3} + \delta r_{4}],$$

$$r_{7} = r_{1} \xi,$$

$$r_{8} = r_{1} \xi e^{-1/T_{R}},$$

$$l_{3} = \frac{e^{1/T_{L}} + \lambda}{r_{1} \xi},$$

$$l_{4} = \frac{\alpha l_{3} \xi \omega + (1 - \beta)e^{1/T_{L}}}{r_{1} \xi},$$

$$l_{5} = l_{6} = e^{1/T_{L}},$$

$$l_{7} = \frac{1 - \lambda}{r_{1} \xi},$$

$$l_{8} = \frac{(1 - \alpha)l_{3} \xi \omega + \beta e^{1/T_{L}}}{r_{1} \xi},$$
(88)

where $\lambda := \alpha - \beta e^{1/T_L}$ and $\mu := \gamma - \delta e^{-1/T_R}$. It is noticeable that, unlike the previous section, the exact solution is obtained without any conditions on the six parameters, α , β , γ , δ , T_L , and T_R . In the high temperature limit $T_L = T_R = \infty$, it agrees with the Bernoulli boundary driving case [9, 11]. In addition, when we set $\alpha = 1 - \beta$, $\gamma = 1 - \delta$, $1/N_L = q_1^L$, and $1/N_R = q_1^R$, the above r's and l's become equal to those in the previous section (55)-(58). Thus the heat-bath boundary condition includes the Bernoulli boundary driving and the conditional boundary driving cases.

3.3. Equilibrium state

When $\alpha = \beta = \gamma = \delta = 0$ and $T_L = T_R = T$, the system is in contact with heat bath at temperature T only. Then, the steady state of the system is considered to be an

equilibrium state at temperature T. We explicitly calculate the probability vector p_s in this case. First, each tensor of PSA is as follows:

$$X = \begin{pmatrix} 1 & 1 & 1 & 1\\ 1 & 1 & e^{-2/T} & e^{-2/T}\\ 1 & 1 & 1 & 1\\ e^{2/T} & e^{2/T} & 1 & 1 \end{pmatrix},$$
(89)

$$L = \begin{pmatrix} 1 & 1 & 1 & 1 \\ e^{1/T} & e^{1/T} & e^{-1/T} & e^{-1/T} \end{pmatrix}, \qquad R = \begin{pmatrix} e^{-1/T} & 1 \\ e^{-1/T} & e^{-2/T} \\ e^{-1/T} & 1 \\ e^{1/T} & 1 \end{pmatrix}.$$
(90)

These can be written in the following form

$$X_{s_2 s_3 s_4 s_5} = \exp\left[2s_3(s_2 - s_4)/T\right],$$

$$L_{s_1 s_2 s_3} = \exp\left[s_1(1 - 2s_2)/T\right],$$

$$R_{s_{n-2} s_{n-1} s_n} = \exp\left[\left(2s_{n-2} s_{n-1} - 2s_{n-1} s_n - 1 + s_n\right)/T\right].$$
(91)

Substituting the three expressions to PSA (25) and rearranging them, we obtain

$$p_{s} = \exp\left[\left(s_{1} + s_{n} - 1 + 2\sum_{i=1}^{n-1} (-1)^{k} s_{i} s_{i+1}\right)/T\right].$$

Because $\sum_{i} E_i = s_1 + s_n + \sum_{i=1}^{n-1} 2(-1)^i s_i s_{i+1}$, the above probability vector represents the equilibrium state at T, as expected.

3.4. Physical quantities in the NESS

Partition function: The exact solution (85)-(88) satisfies the eigenvalue equation,

$$lX = \tau_1 l \qquad X \mathbf{r} = \tau_1 \mathbf{r},$$

$$l'X' = \tau_1 l' \qquad X' \mathbf{r}' = \tau_1 \mathbf{r}',$$
(92)

where

$$\tau_1 = \frac{[\lambda \mu - (1 + e^{1/T_L})(1 + e^{-1/T_R})]^2}{[1 - \lambda \mu + (1 - \mu)e^{1/T_L}][1 - \lambda \mu + (1 - \lambda)e^{-1/T_R}]}.$$
(93)

Then the partition functions are

$$Z_n = \tau_1^{n/2-2} \boldsymbol{l} \cdot \boldsymbol{r}, \qquad Z'_n = \tau_1^{n/2-2} \boldsymbol{l}' \cdot \boldsymbol{r}'. \tag{94}$$

From direct calculation, we find

$$\boldsymbol{l} \cdot \boldsymbol{r} = \boldsymbol{l}' \cdot \boldsymbol{r}' = \frac{(1 + e^{1/T_L})(1 + e^{-1/T_R})}{1 - \lambda \mu + (1 - \mu)e^{1/T_L}} \left[1 - \lambda \mu + (\lambda + 2)e^{-1/T_R} + (\mu + 2)e^{1/T_L} + 3e^{\Delta t} \right]$$
where $\Delta \beta = 1/T_L - 1/T_R \ddagger$, and then $Z_n = Z'_n$.

‡ Do not confuse inverse temperature difference $\Delta\beta$ with left side absorption rate β .

Density: Substituting the exact solution into density definition (66), we obtain

$$\rho_i = \frac{(\lambda + 1)e^{-1/T_R} + (\mu + 1)e^{1/T_L} + 2e^{\Delta\beta}}{1 - \lambda\mu + (\lambda + 2)e^{-1/T_R} + (\mu + 2)e^{1/T_L} + 3e^{\Delta\beta}}.$$
(96)

for $2 \le i \le n-1$. Thus, the density is uniform in this range and the value is denoted as ρ in the following. For i=1 and N, ρ_i can take values different from ρ , but we do not show them because the equations are cumbersome. The temperature dependence of the bulk density is illustrated in Figure 9. Let us check some limiting behavior. For the emission limit α , $\gamma \to 1$, β , $\delta \to 0$ (λ , $\mu \to 1$), the density takes the maximum value 2/3 regardless of temperature parameters. For the absorption limit α , $\gamma \to 0$, β , $\delta \to 1$ ($\lambda \to -e^{1/T_L}$, $\mu \to -e^{-1/T_R}$), it become

$$\rho = \frac{x}{2x+1}, \qquad x = e^{1/T_L} + e^{-1/T_R},$$

and is in the range $0 < \rho \le 1/2$. $\rho = 0$ is established when $1/T_L \to -\infty$, $1/T_R \to \infty$.

In the high temperature limit $T_L, T_R \gg 1$, up to second order of inverse temperatures,

$$\rho \sim \frac{\lambda_0 + \mu_0 + 4}{\lambda_0 + \mu_0 + 8 - \lambda_0 \mu_0} - \frac{1}{(\lambda_0 + \mu_0 + 8 - \lambda_0 \mu_0)^2} \times \left[(\mu_0 + 2)(\alpha \mu_0 + 2\alpha - \lambda_0 - 2) \frac{1}{T_L} - (\lambda_0 + 2)(\gamma \lambda_0 + 2\gamma - \mu_0 - 2) \frac{1}{T_R} \right].$$

Here we have $\lambda_0 = \alpha - \beta$, $\mu_0 = \gamma - \delta$. Furthermore, when the rates of absorption and emission on both boundaries are equal $(\alpha = \gamma, \beta = \delta)$, it becomes

$$\rho \sim \frac{2}{4 - \lambda_0} + \frac{1 - \alpha}{(4 - \lambda_0)^2} \Delta \beta,\tag{97}$$

and depends on the difference of the inverse temperature.

Finally, in the heat conduction limit $\alpha, \beta, \gamma, \delta \to 0$, we have

$$\rho_i = \frac{e^{1/T_L} + e^{-1/T_R} + 2e^{\Delta\beta}}{1 + 2e^{1/T_L} + 2e^{-1/T_R} + 3e^{\Delta\beta}}$$
(98)

for $1 \leq i \leq N$. and in equilibrium $T_L = T_R$, $\rho_i = 1/2$.

Current: Substituting the exact solution into the definition of currents (69), we obtain

$$J_{R} = \frac{\lambda e^{-1/T_{R}} + e^{1/T_{L}} + e^{\Delta \beta}}{1 - \lambda \mu + (\lambda + 2)e^{-1/T_{R}} + (\mu + 2)e^{1/T_{L}} + 3e^{\Delta \beta}},$$

$$J_{L} = \frac{\mu e^{1/T_{L}} + e^{-1/T_{R}} + e^{\Delta \beta}}{1 - \lambda \mu + (\lambda + 2)e^{-1/T_{R}} + (\mu + 2)e^{1/T_{L}} + 3e^{\Delta \beta}}.$$
(99)

The total current is $J = J_R - J_L$. The behavior of the current is illustrated in Figure 10. For the emission limit λ , $\mu \to 1$, the currents become $J_R = 1/3$, $J_L = 1/3$, J = 0 regardless of temperature. For the absorption limit $\lambda \to -e^{1/T_L}$, $\mu \to -e^{-1/T_R}$, it becomes

$$J = \frac{e^{1/T_L} - e^{-1/T_R}}{1 + 2(e^{1/T_L} + e^{-1/T_R})}.$$
(100)

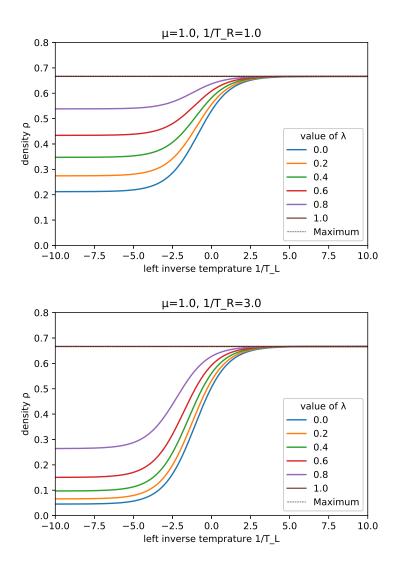


Figure 9. In the case of $\mu=1.0$ and (upper) $1/T_R=1.0$ or (lower) $1/T_R=3.0$, and for different values of λ , we examine the behavior of the bulk density ρ as a function of the inverse temperature $1/T_L$. The maximum density value $\rho=2/3$ is represented by a dotted line, overlapping the $\lambda=1.0$, (thickest) line. Indeed, it can be seen that $\rho=2/3$ regardless of temperature when λ , $\mu=1$. It can also be seen that as $1/T_L$ decreases and $1/T_R$ increases, ρ gets smaller and asymptotically approaches to 0.

In the heat conduction limit, we have

$$J = \frac{e^{1/T_L} - e^{-1/T_R}}{1 + 2(e^{1/T_L} + e^{-1/T_R}) + 3e^{\Delta\beta}}.$$
(101)

It is remarkable that the current does not vanish in equilibrium $(T_L = T_R = T)$ but has a finite value $J = \frac{1}{2} \tanh \frac{1}{2T}$.

Energy: Let us calculate the expectation values of energy and energy flux using the exact NESS solution (85)-(88). Because $|s_i - s_{i+1}| = s_i + s_{i+1} - 2s_i s_{i+1}$, the expectation

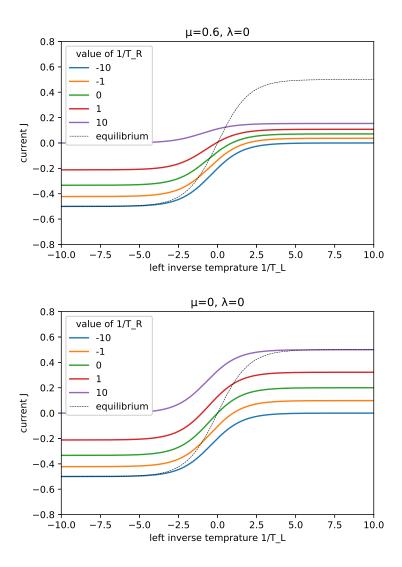


Figure 10. In the case of $\lambda=0$, $(\text{upper})\mu=0.6$ or $(\text{lower})\mu=0$, and for different values of $1/T_R$, we examine the behavior of the bulk current J as a function of the inverse temperature $1/T_L$. The equilibrium current with $\lambda,\mu=0$ and $T_L=T_R$ is represented by a dashed line. Even in the equilibrium state, the particle current generally has a non-zero value as a function of temperature.

value of energy is given as

$$\langle E_{2k} \rangle = 2\rho - 2J_R, \qquad \langle E_{2k+1} \rangle = -2\rho + 2J_L.$$

Because the identity $J_L + J_R = \rho$ holds also in this case, we can write $\langle E_{2k} \rangle = 2J_L$ and $\langle E_{2k+1} \rangle = -2J_R$. The total bulk energy is

$$E = \sum_{k=1}^{n/2-1} (\langle E_{2k} \rangle + \langle E_{2k+1} \rangle) = -(n-2)J.$$
 (102)

Since the NESS vector does not depend on time, we can see immediately that the

expectation value of energy flux is

$$\langle S_i \rangle = 1 - 2\rho = \frac{1 - (\lambda + e^{1/T_L})(\mu + e^{-1/T_R})}{1 - \lambda\mu + (\lambda + 2)e^{-1/T_R} + (\mu + 2)e^{1/T_L} + 3e^{\Delta\beta}}.$$
 (103)

Thus, if the condition $(\lambda + e^{1/T_L})(\mu + e^{-1/T_R}) = 1$ or

$$[\alpha + (1 - \beta)e^{1/T_L}][\gamma + (1 - \delta)e^{-1/T_R}] = 1$$
(104)

holds, the energy current vanishes and the bulk density of 1 is 1/2. Under this condition, the matrices X, R, and L are

$$X = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & \phi^{-2} & \phi^{-2} \\ 1 & 1 & 1 & 1 \\ \phi^2 & \phi^2 & 1 & 1 \end{pmatrix}$$
 (105)

$$L = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \phi - \lambda & \phi - \lambda & 1 - \lambda & 1 - \lambda \end{pmatrix}, \tag{106}$$

$$R = \begin{pmatrix} \phi^{-1} & 1 - \mu \\ \phi^{-1} & \phi^{-2}(1 - \mu\phi) \\ \phi^{-1} & 1 - \mu \\ \phi & 1 - \mu\phi \end{pmatrix}$$
(107)

where $\phi := \lambda + e^{1/T_L}$. Thus we can represent the solution with only three parameters ϕ , λ and μ . Note that X, the first row of L, and the first column of R are the same as those of the equilibrium state at $T = (\log \phi)^{-1}$. Parameters in the partition function, $l \cdot r$ and τ_1 are also simplified to

$$\boldsymbol{l} \cdot \boldsymbol{r} = \frac{2N_L N_R (1+\phi)}{\phi}, \quad \tau_1 = \frac{(1+\phi)^2}{\phi}$$
 (108)

The densities at the boundary cells are obtained as

$$\rho_1 = \frac{2N_L - 1 - \phi}{2N_L}, \quad \rho_n = \frac{2N_R - 1 - \phi^{-1}}{2N_R}.$$
 (109)

The currents J_L and J_R are

$$J_L = \frac{1}{2(1+\phi)}, \quad J_R = \frac{\phi}{2(1+\phi)}, \quad J = \frac{\phi-1}{2(1+\phi)}.$$
 (110)

Thus the steady states in this case is the same as the equilibrium one at temperature $T = (\log \phi)^{-1}$ except the density at the boundary cells. Such a state is illustrated in Figure 11, where we see more lines downward to the right than those to the left. In the limit $\lambda, \mu \to 0$, the solutions approach the equilibrium ones.

In the high temperature limit, if the absorption and release rates at both boundaries are equal, the energy flux become

$$\langle S_i \rangle \sim \frac{\lambda_0}{4 - \lambda_0} - \frac{2(1 - \alpha)}{(4 - \lambda_0)^2} \Delta \beta,$$
 (111)

and depend only on the temperature difference of the thermal baths at both ends. In particular, if the emission and absorption rates are equal $(\alpha = \beta)$, we see that $\langle S_i \rangle \sim (1 - \alpha)(T_L - T_R)/(8T_L T_R)$.



Figure 11. A nonequilibrium steady state without energy flow. Parameter values are $(\alpha, \beta, \gamma, \delta) = (0.8, 0.2, 0.1875, 0.75), e^{1/T_L} = 4.0$, and $e^{-1/T_R} = 0.25$.

4. Discussion

We have obtained two generalizations of Prosen and Mejía-Monasterio's result on nonequilibrium steady states of RCA54. One is achieved by extending the probabilities for the states of the virtual stochastic cells at the boundaries. In [9], the cells take values 0 or 1 with probability 1/2. We have generalized it to ζ and $1-\zeta$ for the left boundary and η and $1-\eta$ for the right boundary. The patch state ansatz has been successfully applied to construct nonequilibrium steady states on the assumption (48) for the absorption and emission rates. Actually this boundary condition is equivalent to the conditional boundary driving case studied in [11] using a different method. Our solution takes a different form from that in [11]. We expect that they are consistent with each other, but could not verify it due to complexity of the latter solution.

The other is obtained by regarding an additive conserved quantity of RCA54 as energy and employing Boltzmann weights as the probabilities for the virtual cells. Such a boundary condition is originated from the study of ERCAs by one of the authors. Under this boundary condition, the system can be regarded as in contact with heat reservoirs and the temperatures of the left and right reservoirs are introduced to the model. Thus we can consider two kinds of motion in this model: One is the motion of particles and the other is that of energy. We think that the latter is more physical because it is based on a conservation law. Equilibrium states are also naturally introduced at any temperature as the steady states in the case that both the temperatures are equal and no absorption or emission occurs. Properties of energy transport is also studied if the two reservoirs have different temperature values. The exact solution in the heat-bath boundary case has been derived for any set of the parameters without any additional conditions on absorption or emission rates. Moreover, this boundary condition includes the Bernoulli boundary driving and the conditional boundary driving as limiting cases. Thus, the heat-bath boundary condition unifies all the known solvable cases of RCA54.

The exact solutions obtained exhibit uniform density of 1 in the bulk and ballistic transport. In the first solution, the current of particles is approximately proportional to $\gamma - \alpha$ if $\eta = \zeta$ and difference between α and γ is small. The second solution has a richer structure, where there exist heat-bath temperature and the energy current besides the particle current. We have discussed density profile, particle current, energy and energy current in a variety of limiting cases. The particle current exists even in equilibrium states, where energy current vanishes. It is no wonder because the number of particles is not a conserved quantity in this system. We have explicitly derived the condition for vanishing energy current. Interestingly, it contains the case with finite emission and absorption rates, where only the end cells 1 and n show density different from equilibrium state at effective temperature ($\log \phi$)⁻¹.

The present method may be further extended to other CA rules. In ERCA, there are a number of rules that show various types of nonequilibrium steady states. Some rules show flat density profile and ballistic transport like RCA54, some others show a nonzero density gradient near the boundaries and still ballistic transport, and some others show a global density gradient and diffusive behavior with respect to a certain additive conserved quantity. It will be interesting to examine whether the present method can be generalized to such rules. It is a future problem.

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