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

Atsuo Inoue and Shinji Takesue

Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan
E-mail: inoue.atsuo.26u@st.kyoto-u.ac.jp and takesue@scphys.kyoto-u.ac.jp

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Abstract
Recently Prosen and Mejia-Monasterio (2016 J. Phys. A: Math. Theor. 49 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 obtained by generalizing probabilities for values of virtual cells while imposing a special condition on emission and absorption rates. Although this actually coincides with the conditional boundary driving discussed in Prosen and Buča (2017 J. Phys. A: Math. Theor. 50 395002), we present a solution in a different form. The other is obtained by considering a conserved quantity as energy, and by considering boundaries as heat reservoirs. The latter contains the original solution and the former one as the special cases. Properties of both solutions are discussed.

Keywords: cellular automaton, nonequilibrium steady state, integrability, Markov chain

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 have not only been 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 a one-dimensional reversible CA of the form [5–7]

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

(1)
where \(i\) and \(t\) denote integers representing the cell and time, respectively, \(x_i^t \in \{0, 1\}\) means the state of cell \(i\) at time \(t\), and \(\oplus\) is 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

\[
x_i^{t-1} = f(x_{i-1}^t, x_i^t, x_{i+1}^t) \oplus x_{i+1}^{t+1}.
\]

This type of CA is the second-order variant of Wolfram’s elementary CA, and thus is called the elementary reversible CA (ERCA). Each rule is referred to as Wolfram’s code \(\sum x, y, z = 0, 1\) \(f(x, y, z) = 1\) appended by an ‘R’. For example, if \(f(000) = f(010) = 0\) and \(f(x, y, z) = 1\) for other configurations, the rule is called 250R. Due to the discrete nature of the 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 the 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 the 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, transport of energy occurs. 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 Mejia-Monasterio [9] proposed a similar reversible CA model with stochastic boundary conditions that represents chemical baths for absorbing and emitting particles. Their model is based on rule 54 (RCA54) presented by Bobenko et al [10]; the rule is defined on a one-dimensional zigzag chain. At first glance, ECA54 is different from the ERCA, but it is related to rule 250R in the ERCA, as we will see afterward. Prosen and Mejia-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 (PSA). This is the first time that an exact NESS has been 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 Bernoulli driving in [11]; the other is called 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 Mejia-Monasterio’s method by devising novel boundary conditions for the same model as in [9, 11]. 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 using the PSA in a different form from that given in [11]. The other generalization is obtained by employing the heat bath boundary conditions, which was originally devised for ERCA. We will show 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 a summary and discussion.
2. Boundary-driven CA model

2.1. Definitions

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

RCA54 is a one-dimensional discrete system that consists of cells connected in a zigzag chain, as shown in figure 1. Each cell takes a value of zero or one. 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:

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

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

where $s_i^t \in \{0, 1\}$ 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

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

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

$$\chi(s, s', s'') = t \iff \chi(s, t, s'') = s',$$ (6)

which means that the CA is time-reversal invariant. The Wolfram code for this $\chi$ is 54, and therefore this CA is called RCA54. It should be noted that there is no relation to Wolfram’s elementary CA or ERCA with the same code number.

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

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 both ends of the system. The value of the 0th cell is given as $s_0^{t+1} = 0$ with probability $\zeta$, and $s_0^{t+1} = 1$ with $1 - \zeta$. Similarly, the value of the $(n + 1)$st cell is given as $s_{n+1}^{t+1} = 0$ with probability $\eta$, 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 the emission and absorption of particles at the boundaries as follows. If $s_i^t = 0$ at time $t$, we change it to $s_i^t = 1$ with probability $\alpha$, which corresponds to emission. Similarly, if $s_i^t = 1$ at time $t$, we change it to $s_i^t = 0$ with probability $\beta$, which corresponds to absorption (figure 5).

Thus, in RCA54, the bulk is deterministically developed and the boundary is stochastically developed. A configuration at time $t$ is represented by a binary sequence $s^t = s_1^t, s_2^t, \ldots, s_n^t$. 

Figure 1. Illustration of a configuration of our system composed of 12 diamond-shaped cells. Each cell takes a value of zero (white) or one (black). This figure represents the configuration 011001001101.
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 \( p_t^s \) be the probability of taking configuration \( s \) at time \( t \). The state of the system at time \( t \) is given by state vector \( p_t^s = (p_t^0, p_t^1, \ldots, p_t^{2^n-1}) \), which evolves in time according to the master equation of the form

\[
p_t^s + 1 = U p_t^s,
\]

or

\[
p_t^{s+1} = \sum_{s'} U_{ss'} p_t^{s'}.
\]

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

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 zero. Values of one are colored black, and move to the left or right with velocity \( \pm 1 \) until collision occurs. When two particles collide, they shift to the next lower cell and then separate.

Because each configuration corresponds one-to-one to the binary number of \( n \) digits, the total number of configurations is \( 2^n \).

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 \( s = s_1 \cdots s_n \) and that at time \( t + 1 \) be \( u = u_1 \cdots u_n \). Then, step (i) changes configuration \( s \) to...
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 $0 < \alpha, \beta, \gamma, \delta < 1$.

Figure 6. Separation of time evolution. $U_e$ and $U_o$ are transition matrices corresponding to steps (i) and (ii), respectively.
s_1u_2s_3u_4 \cdots u_n$, which is transformed into $u$ by step (ii) (see figure 6). It is noted that in step (i) $u_2$ is determined only from the three values $s_{2k-1}$, $s_{2k}$, and $s_{2k+1}$, and $u_0$ is probabilistically chosen depending on $s_{n-1}$ and $s_n$. Each transition is represented by small transition matrices as follows.

The transition from $s_{2k-1}s_{2k}s_{2k+1}$ to $s_{2k-1}u_2s_{2k+1}$ is given by (3). Interpreting this transition as a three-digit binary number to a three-digit binary number, the local transition matrix is written using the following $8 \times 8$ matrix

\[
P = \begin{pmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1 \\
\end{pmatrix},
\]

or tensor

\[
P_{uu'u'}|ss's'' = \delta_{uu'}\delta_{s}'(s,s')\delta_{s''},
\]

\[
(9)
\]

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

Next we consider the effect of virtual cell 0 on the left boundary block $s_1u_2$. When cell 0 takes value $u_0 = 0$, which occurs with probability $\zeta$, the upper left half of the matrix $P$ acts on $s_1u_2$. If $u_0 = 1$, which occurs with probability $1 - \zeta$, the lower right half of $P$ acts on $s_1u_2$. Thus, the transition matrix on the left boundary cells $s_1s_2$ is

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

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

\[
\tilde{P}^R = \begin{pmatrix}
\eta & 1 - \eta \\
1 - \eta & \eta \\
\end{pmatrix}.
\]

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

\[
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\]

\[
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\]
$$P^L = \tilde{P}^L(1_2 \otimes B^L) = \begin{pmatrix} q^L_1 & 1 - q^L_2 \\ 1 - q^L_1 & 1 - \alpha \end{pmatrix},$$  
$$(13)$$

$$P^R = \tilde{P}^R(B^R \otimes 1_2) = \begin{pmatrix} q^R_1 & 1 - q^R_2 \\ 1 - q^R_1 & \gamma \end{pmatrix},$$  
$$(14)$$

Here, $1_2$ is a $2 \times 2$ unit matrix, and

$$q^L_1 = \zeta + \alpha - 2\zeta\alpha, \quad q^L_2 = \zeta + \beta - 2\zeta\beta,$$  
$$(15)$$

$$q^R_1 = \eta + \gamma - 2\eta\gamma, \quad q^R_2 = \eta + \delta - 2\eta\delta.$$  
$$(16)$$

Since $0 \leq \alpha, \beta, \gamma, \delta, \zeta, \eta \leq 1$, these parameters also satisfy $0 \leq q^L_1, q^L_2, q^R_1, q^R_2 \leq 1$.

The transition matrix $U$ can be written as

$$U = U_0 U_e,$$  
$$(17)$$

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

$$U_o = P_{12} P_{234} P_{456} P_{678} \cdots P_{n-2,n-1,n},$$  
$$(19)$$

where

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

and

$$p^L_{12} = P^L_1 \otimes 1_{2^{n-i}}, \quad p^L_{n-1,n} = 1_{2^{n-i}} \otimes p^R.$$  
$$(21)$$

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. NESS

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

$$p = U p$$  
$$(22)$$

or

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

These equations mean that $p$ is an eigenvector with eigenvalue 1 of the transition matrix $U$. We refer to (23) as an NESS equation, and to $p_s$ that satisfies (22) as an NESS vector. The existence and uniqueness of the NESS is guaranteed by the 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 \((U^t)_{ss} > 0\) 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 Perron–Frobenius’s theorem, when \(U\) is irreducible and aperiodic, the maximum eigenvalue of a stochastic matrix is one and its eigenspace is one dimension \([12]\). Thus, the solution of the NESS equation (23) is unique.

We divide the master equation into

\[
p_s = \sum_{s'} (U_s)_{ss'} p_{s'}, \quad p_s' = \sum_{s'} (U_s')_{ss'} p_{s'},
\]

and assume from the following PSA that the solution can be written in the form

\[
p_s = L_{s1} L_{s2} L_{s3} L_{s4} L_{s5} L_{s6} \cdots X_{s_{n-1} s_{n-2} s_{n-3} s_{n-4} s_{n-5} s_{n-6} \cdots} R_{s_{n-1} s_{n-2} s_{n-3} s_{n-4} s_{n-5} s_{n-6} \cdots},
\]

\[
p_s' = L_{s1}' L_{s2}' L_{s3}' L_{s4}' L_{s5}' L_{s6}' \cdots X_{s_{n-1}' s_{n-2}' s_{n-3}' s_{n-4}' s_{n-5}' s_{n-6}' \cdots} R_{s_{n-1}' s_{n-2}' s_{n-3}' s_{n-4}' s_{n-5}' s_{n-6}' \cdots}.
\]

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.

2.3.1 Normalizations. When the configuration is a vacuum state \(s = 0 \cdots 0\), (25) and (26) are

\[
p_{0 \cdots 0} = L_{000}(X_{0000})^{n/2-2} R_{000}, \quad p_{0 \cdots 0}' = L_{000}'(X_{0000}')^{n/2-2} R_{000}'.
\]

\(U_s\) can change the value of cell \(n\) and the \(U_o\) value of cell 1, but the rest remains 0. Hence,

\[
L_{000}(X_{0000})^{n/2-2} R_{000} = \sum_{s_n} (U_s)_{0 \cdots 0} L_{000}'(X_{0000}')^{n/2-2} R_{000}'.
\]

Since this is true even if \(n\) changes to \(n + 2\), we can see by taking the ratio of the two equations that

\[
X_{0000} = X_{0000}'.
\]

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

2.3.2 Gauge symmetry. PSAs (25) and (26) have gauge symmetry, which makes the equation invariant. Let \(f_{st}, f_{st}'\) be arbitrary 2-tensors. The NESS equation is then invariant under the following gauge transformation:

\[
X_{st} X_{st}' \mapsto f_{st} X_{st} f_{st}'^{-1},
\]

\[
L_{st} \mapsto L_{st} f_{st}^{-1},
\]

\[
R_{st} \mapsto f_{st} R_{st},
\]

\[
X_{st}' X_{st} \mapsto f_{st}' X_{st} f_{st}'^{-1},
\]

\[
L_{st}' \mapsto L_{st} f_{st}'^{-1},
\]

\[
R_{st}' \mapsto f_{st} R_{st}'.
\]
If we fix the gauge to
\[ f_{ss'} = (L_{000}, X_{0001}, X_{0010}, X_{0011}), \]
\[ f_{ss'}' = (R_{000}^{-1}, X_{0001}', X_{0010}', X_{0011}'), \]
we can transform the PSA components into
\[ L_{000}, R_{000}', X_{0001}', X_{0010}', X_{0011}' \rightarrow 1. \]
Note that under this gauge transformation, the diagonal components are invariant, \( X_{ss'} \rightarrow f_{ss} X_{ss'} f_{ss}^{-1} = X_{ss'}' \).

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, the PSA gives the unique solution.

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

\[
X = \begin{pmatrix}
1 & 1 & 1 & 1 \\
y_1 & y_2 & y_3 & y_4 \\
y_5 & y_6 & y_7 & y_8 \\
y_9 & y_{10} & y_{11} & y_{12}
\end{pmatrix},
\]
\[
X' = \begin{pmatrix}
1 & 1 & 1 & 1 \\
y_1' & y_2' & y_3' & y_4' \\
y_5' & y_6' & y_7' & y_8' \\
y_9' & y_{10}' & y_{11}' & y_{12}'
\end{pmatrix}.
\]

Similarly, \( L_{ss''}, L'_{ss''} \) and \( R_{ss''}, R'_{ss''} \) can be represented using \( 2 \times 4, 4 \times 2 \) matrices, respectively:

\[
L = \begin{pmatrix}
1 & l_2 & l_3 & l_4 \\
l_5 & l_6 & l_7 & l_8
\end{pmatrix}, \quad L' = \begin{pmatrix}
l_1' & l_2' & l_3' & l_4' \\
l_5' & l_6' & l_7' & l_8'
\end{pmatrix},
\]
\[
R = \begin{pmatrix}
r_1 & r_2 \\
r_3 & r_4 \\
r_5 & r_6 \\
r_7 & r_8
\end{pmatrix}, \quad R' = \begin{pmatrix}
r_1' & r_2' \\
r_3' & r_4' \\
r_5' & r_6' \\
r_7' & r_8'
\end{pmatrix}.
\]

2.3.4. 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 \( s_1 \), \( s_2 \), and \( s_3 \) are 0; (ii) all indices except \( s_{n-2} \), \( s_{n-1} \), and \( s_n \) are 0; and (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, by calculating the NESS equation (23) directly we obtain

\[
L'_{ss',00} X'_{ss',00} = \sum_{k} (P^R)_{000} L_{ss',00}^R X_{ss',s_k} X_{s_k,s_0} X_{s_0,00},
\]

\[ (39) \]
In (43) and (44), we replaced $s_{2k+2}, s_{2k+3}, s_{2k+4}, s_{2k+5}$ by $s_{2} s_{3} s_{4} s_{5}$ for simplicity of presentation. Solving these equations, we have

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

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

$$L = \begin{pmatrix} 1 & l_2 & l_3 & l_4 \\ l_5 & l_6 & l_7 & l_8 \end{pmatrix}, \quad L' = \begin{pmatrix} l'_1 & l'_4 & l'_5 & l'_6 \\ l'_1 l_2 / y_1 & l'_1 l_5 & l'_1 l_6 \end{pmatrix},$$

$$R = \begin{pmatrix} r_1 & r_2 \\ r_3 & r_4 \\ r_5 & r_6 \\ r_7 & r_8 \end{pmatrix}, \quad R' = \begin{pmatrix} 1 & r_4 / r_1 \\ r_3 / r_1 & r_2 / r_1 \\ y_3 y_5 r_7 / r_5 & y_3 y_5 r_8 / r_5 \\ r_5 / (y_3 r_1) & r_6 / (y_3 r_1) \end{pmatrix}.$$
\[ r_1 = t_1^\prime q_1^l + (1 - q_1^l_k) l_1 y_1, \]
\[ r_1 l_2 = t_1^\prime [q_1^l l_4 + (1 - q_1^l_k) l_6], \]
\[ r_1 l_3 = t_1^\prime y_1 [\alpha l_2 + (1 - \beta) l_6], \]
\[ r_1 l_4 = t_1^\prime y_3 [\alpha l_1 y_1 + (1 - \beta) l_5], \]
\[ r_1 l_5 = t_1^\prime [1 - q_1^l + q_1^l_k l_2 y_1], \]
\[ r_1 l_6 = t_1^\prime [(1 - q_1^l_k) l_4 + q_1^l_k l_8], \]
\[ r_1 l_7 = t_1^\prime y_3 [1 - \alpha l_2 + \beta l_6], \]
\[ r_1 l_8 = t_1^\prime y_4 / y_1 [(1 - \alpha) l_3 y_1 + \beta l_3]. \]  

(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 zero, (vi) all indices except \( s_{n-4}, s_{n-3}, s_{n-2}, s_{n-1}, (k = n/2 - 3)\) are zero. From these components, we obtain the following equations:

\[ y_2 = y_1, \]
\[ y_4 = y_1 y_3, \]
\[ t_1^\prime y_1 = q_1^l R_5 + (1 - q_1^l_k) R_6, \]
\[ t_1^\prime y_3 = q_1^l R_1 + (1 - q_1^l_k) R_2, \]
\[ r_1 = t_1^\prime [q_1^l l_4 + (1 - q_1^l_k) l_6], \]
\[ r_1 l_2 = t_1^\prime [q_1^l + (1 - q_1^l_k)] l_2 y_1]. \]  

(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 \( y_1, y_3, l_3, ..., l_8, r_1, ..., r_8, \) and \( t_1^\prime \). Because all components of \( R \) and \( L' \) include \( t_1^\prime \) as a factor, and the PSA also does, we can set \( t_1^\prime = 1 \) by using the freedom of multiplying a constant to the eigenvector.

2.3.5. 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 \( \zeta \) and \( \eta \) if the conditions

\[ \alpha = 1 - \beta, \quad \gamma = 1 - \delta \]  

(48)

are satisfied. When these conditions are satisfied, the probability of \( s_1 = 1 \) is \( \alpha \) and that of \( s_n = 1 \) is \( \gamma \) irrespective of the previous values of \( s_1 \) and \( s_n \). Both cases are united into \( q_1^l = 1 - q_1^l_k \) and \( q_1^R = 1 - q_1^R_k \), 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

\[ P^L = \begin{pmatrix}
q_1^l & \alpha \\
1 - q_1^l & 1 - \alpha
\end{pmatrix}, \quad
P^R = \begin{pmatrix}
\alpha & q_1^l \\
1 - \alpha & 1 - q_1^l
\end{pmatrix}. \]  

(49)
$P^R = \begin{pmatrix} q_1^R & q_1^R \\ 1 - q_1^R & 1 - q_1^R \\ \gamma & \gamma \\ 1 - \gamma & 1 - \gamma \end{pmatrix}. \quad (50)$

These boundary stochastic matrices actually operate on the states of cells one and two without referring to the virtual cells zero and $n + 1$. For example, the above $P_L$ means that cell one at the next time takes zero with probability $q_1^L$ if $s_2 = 0$ and with probability $\alpha$ if $s_2 = 1$. Thus, these are essentially equivalent to the conditional driving boundary conditions in [11]: $q_1^L$ and $\alpha$ in (49) correspond to $\alpha$ and $\beta$ in equation (13) of [11], respectively; $q_1^R$ and $\gamma$ in (50) correspond to $\gamma$ and $\delta$ in [11], respectively. The only difference is that $q_1^L$ and $q_1^R$ depend on $\alpha$ and $\gamma$ 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

\begin{align*}
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), \quad (51)
\end{align*}

\begin{align*}
r_1 &= q_1^L (1 + l_2 y_1), \\
r_7 &= q_1^L (l_4 + l_5), \\
r_1 l_3 &= y_3 \alpha (1 + l_5), \\
r_1 l_4 &= y_3 \alpha (l_3 y_1 + l_5), \\
r_1 l_5 &= (1 - q_1^L) (1 + l_2 y_1), \\
r_1 l_6 &= (1 - q_1^L) (l_4 + l_5), \\
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), \\
r_2 &= r_1 / y_3. \quad (52)
\end{align*}

We then arrive at the same form of transfer matrices as in equation (43) in [9]:

\begin{align*}
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}, \\
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}. \quad (54)
\end{align*}
\[ \xi := \frac{1}{\gamma_3} \left[ (1 - \gamma)\alpha + (1 - \alpha)q_1^R \right] \left( (\alpha + (1 - \alpha)q_1^R - q_1^L q_1^R) \right), \]  
\[
\omega := \gamma_3 \left[ (1 - \gamma)\gamma + (1 - \gamma)q_1^L \right] \left( (\gamma + (1 - \gamma)q_1^L - q_1^L q_1^R) \right). \]

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

\[
\begin{align*}
    r_1 &= \frac{(1 - \alpha)\gamma + (1 - \gamma)q_1^L}{(1 - \gamma)\alpha + (1 - \alpha)q_1^R}, \\
    r_2 &= \frac{1 - \gamma}{q_1^R[(1 - \gamma)\alpha + (1 - \alpha)q_1^R]} \left( (\alpha + (1 - \alpha)q_1^R - q_1^L q_1^R) \right), \\
    r_3 &= \frac{\gamma}{q_1^R[(1 - \gamma)\alpha + (1 - \alpha)q_1^R]} \left( (\alpha + (1 - \alpha)q_1^R - q_1^L q_1^R) \right), \\
    r_4 &= \left( \frac{1}{q_1^R} - 1 \right) \frac{(1 - \alpha)\gamma + (1 - \gamma)q_1^L}{(1 - \gamma)\alpha + (1 - \alpha)q_1^R}, \\
    r_5 &= \frac{\gamma}{q_1^R[(1 - \gamma)\gamma + (1 - \gamma)q_1^L][1 - (1 - \gamma)\alpha + (1 - \alpha)q_1^R]} \left[ (\alpha + (1 - \alpha)q_1^R - q_1^L q_1^R) \right], \\
    r_6 &= \frac{1 - \gamma}{q_1^R[(1 - \gamma)\gamma + (1 - \gamma)q_1^L][1 - (1 - \gamma)\alpha + (1 - \alpha)q_1^R]} \left[ (\alpha + (1 - \alpha)q_1^R - q_1^L q_1^R) \right], \\
    r_7 &= \frac{\gamma}{q_1^R[(1 - \gamma)\gamma + (1 - \gamma)q_1^L][1 - (1 - \gamma)\alpha + (1 - \alpha)q_1^R]} \left[ (\alpha + (1 - \alpha)q_1^R - q_1^L q_1^R) \right], \\
    r_8 &= \left( \frac{1}{q_1^R} - 1 \right) \frac{(1 - \alpha)\gamma + (1 - \gamma)q_1^L}{(1 - \gamma)\gamma + (1 - \gamma)q_1^L}, \\
    l_3 &= \frac{\alpha}{q_1^L\alpha + (1 - \alpha)q_1^L}, \\
    l_4 &= \frac{\alpha}{q_1^L(1 - \gamma)\alpha + (1 - \alpha)q_1^L}, \\
    l_5 &= l_6 = \frac{1}{q_1^R} - 1, \\
    l_7 &= \frac{1 - \alpha}{q_1^L\alpha + (1 - \alpha)q_1^L}, \\
    l_8 &= \frac{1 - \alpha}{q_1^L(1 - \gamma)\alpha + (1 - \alpha)q_1^L}, \\
\end{align*}
\]

2.4. Physical quantities in the NESS

2.4.1. Partition function. Since the NESS vectors \( p_s, p'_s \) are obtained, we can calculate the expectation values of physical quantities with these vectors. Partition functions of the system are
\[ Z_n := \sum_s p_s, \quad Z'_n = \sum_s p'_s. \]  
(59)

Substituting PSAs (25) and (26) into (59) gives the following matrix product forms:

\[ Z_n = IX^{n/2-2}r, \quad Z'_n = I'X^{n/2-2}r'. \]  
(60)

Here we introduced four component vectors:

\[ l := (L_{0s} + L_{1s'}), \quad l' := (L'_{0s} + L'_{1s'}), \]
\[ r := (R_{s0} + R_{ss'}), \quad r' := (R'_{s0} + R'_{ss'}). \]  
(61)

In the case of an exact solution (55)–(58), the following are satisfied:

\[ IX = \tau_l l, \quad Xr = \tau_r r, \]
\[ l'X' = \tau'_l l', \quad X'r' = \tau'_r r'. \]  
(62)

That is, \( l \) and \( r \) are eigenvectors of \( X \) belonging to the eigenvalue \( \tau_l \). By using this fact repeatedly,

\[ Z_n = \tau_n^{n/2-2} l \cdot r, \quad Z'_n = \tau'_n^{n/2-2} l' \cdot r'. \]  
(64)

From direct calculation, we obtain

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

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

**2.4.2. Density.** We define the density of one at cell \( i \) as

\[ \rho_i := \frac{1}{Z_n} \sum_s s_ip_s. \]  
(66)

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

\[ \rho_{2k} = \frac{1}{Z_n} \sum_{s_k, s_{k+1}} (IX^{k-1})_{s_{2k}, s_{2k+1}} s_{2k} X^{n/2-k-1}r_{2k, 2k+1}. \]

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

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

Substituting the exact solution, we arrive at

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

Similarly, we can derive \( \rho_{2k+1} = \rho_{2k} \) for \( k = 1, \ldots, n/2 - 1 \). Thus, the density of one is uniform in \( 2 \leq i \leq n - 1 \) and its value is denoted by \( \rho \) in the following.
Finally, unlike bulk, the densities at boundary \( i = 1, n \) are calculated by the formulas

\[
\rho_1 = \frac{\tau_{n/2-2}}{Z_n} \sum_{\delta_1, \delta_2} I_{\delta_1, \delta_2}, \\
\rho_n = \frac{\tau_{n/2-2}}{Z_n} \sum_{\delta_{n-2}, \delta_n} I_{\delta_{n-2}, \delta_n} R_{\delta_{n-2}, \delta_n-1} \tag{68}
\]

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

Let us examine the range of values for the bulk density. For the emission limit \( \alpha, \gamma \to 1 \), the density takes the maximum value \( 2/3 \) regardless of \( \zeta, \eta \). However, for the absorption limit \( \alpha, \gamma \to 0 \), it becomes

\[
\rho = \frac{2-x}{3-2x}, \quad x = \frac{1}{\zeta} + \frac{1}{\eta}.
\]

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 \( \delta_{2k} = \delta_{2k+1} = 1 \) only in the case \( \delta_{2k-1} = 0 \), which inevitably leads to \( \delta_{2k+1} = 1 \) because \( \chi(\ast, 0, 1) = \chi(1, 0, \ast) = 1 \). Then, \( \delta_{2k}^+ = \chi(\delta_{2k-1}, \delta_{2k}, \delta_{2k+1}) = \chi(1, 1, 1) = 0 \). Thus, any cell cannot have 1 three times in a row. Therefore, the density of one 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].

### 2.4.3. Current

As in [9, 10], 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

\[
J_R := \frac{1}{Z_n} \sum_s s_{2k} s_{2k+1} P_2, \\
J_L := \frac{1}{Z_n} \sum_s s_{2k+1} s_{2k+2} P_2. \tag{69}
\]

By substituting the PSA (25) and using (62), \( J_R \) is obtained as

\[
J_R = \frac{\tau_{n/2-2}}{Z_n} \sum_{s_{2k}, s_{2k+1}} I_{s_{2k}, s_{2k+1}} \sum_r R_{s_{2k}, s_{2k+1}} R_{s_{2k+1}} \bigg| q_1^R + q_1^R q_1^R \bigg| \frac{\alpha - (1 - \alpha)q_1^R}{\alpha \gamma - 2\alpha - 2\gamma - 2(1 - \alpha)q_1^R - 2(1 - \gamma)q_1^R + 3q_1^R q_1^R}. \tag{70}
\]

Quite similarly, \( J_L \) is obtained as

\[
J_L = \frac{\tau_{n/2-2}}{Z_n} \sum_{s_{2k}, s_{2k+1}} I_{s_{2k}, s_{2k+1}} \sum_r R_{s_{2k}, s_{2k+1}} R_{s_{2k+1}} \bigg| q_1^R + q_1^R q_1^R \bigg| \frac{\eta - (1 - \gamma)q_1^R}{\alpha \gamma - 2\alpha - 2\gamma - 2(1 - \alpha)q_1^R - 2(1 - \gamma)q_1^R + 3q_1^R q_1^R}. \tag{71}
\]

Thus, we arrive at

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

\[15\]
In the case where $\eta = \zeta$ and the difference between $\alpha$ and $\gamma$ is small, the current is approximately proportional to $\gamma - \alpha$.

We notice another interesting relation

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

This is also explained in the same manner as for the maximum value of the bulk density. Assume $(s'_{2k-1}, s'_{2k}, s'_{2k+1}) = (0, 1, 0)$. Then, $s'_{2k+1} = \chi(s'_{2k-1}, s'_{2k}, s'_{2k+1}) = 1$, and because $\chi(0, 1, 0) = 1$, we have $s'_{2k-1} = s'_{2k} = 1$ and $s'_{2k+1} = \chi(s'_{2k-1}, s'_{2k}, s'_{2k+1}) = 1$, namely we obtain $(s'_{2k-1}, s'_{2k}, s'_{2k+1}) = (1, 1, 1)$. The time-reversal symmetry of the rule (6) ensures that the inverse is true; if $(s'_{2k-1}, s'_{2k}, s'_{2k+1}) = (1, 1, 1)$, we have $(s'_{2k-1}, s'_{2k}, s'_{2k+1}) = (0, 1, 0)$. Similarly, we can derive $(s'_{2k-1}, s'_{2k}, s'_{2k+1}) = (0, 1, 0)$ if and only if $(s'_{2k}, s'_{2k+1}, s'_{2k+2}) = (1, 1, 1)$. These properties lead to the fact that the marginal distribution $p(s_{-1}, s_i, s_{+1})$ in a stationary state must satisfy $p(0, 1, 0) = p(1, 1, 1)$ for $2 \leq i \leq N - 2$. 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 $\rho_0 = p(0, 1, 0) + p(1, 1, 0) + p(0, 1, 1) + p(1, 1, 1)$. Thus, the relation (73) is derived from $p(0, 1, 0) = p(1, 1, 1)$. This relation must be satisfied in all stationary states.

3. Temperature-driven reversible CA 54

3.1. The relation between RCA 54 and ERCA 250R

Before introducing the boundary condition, we discuss the relation between Bobenko’s RCA 54 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

$$x^+_{i} = x^i \oplus x^i_{+1} \oplus x^i_{-1} \oplus x^i_{+1} \oplus x^i_{-1},$$  \hfill (74)

where we have changed $i$ to $\tau$. It should be noted that the right-hand side of this equation does not depend on $x^i_{\tau}$. This property leads to the fact that spatiotemporal evolution $\{x^i_{\tau}\}$ with $i + \tau = \text{even}$ and that with $i + \tau = \text{odd}$ are independent of each other. In the former set, if we write $s^i_{2k} = x^i_{2k}$ and $s^i_{2k+1} = x^i_{2k+1}$, $s^i_{2k+1}$ is determined by (3) and $s^i_{2k+1}$ is determined by (4). The set $\{x^i_{\tau}\}$ with $i + \tau = \text{odd}$ is similarly regarded as the evolution of RCA 54. That is, ERCA rule 250R is decomposed into two independent RCA 54. This is illustrated in figure 7.

3.2. Heat bath boundary conditions

We introduce here a heat bath boundary condition to RCA 54 in the same manner as is done in [7] for ERCA. To do so, we have to identify an additive conserved quantity for RCA 54. It is shown in [8] that ERCA rule 250R has several such conserved quantities. We adapt the result to RCA 54 and obtain the following:

$$E^i_{\tau} := (-1)^{i+1} |s^i_{\tau} - s^i_{\tau+1}| = \begin{cases} (-1)^{i+1} & s_i \neq s_{i+1} \\ 0 & s_i = s_{i+1} \end{cases}. \hfill (75)$$

This is a conserved density, and 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 $\chi$: 

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\[ |x - y| - |y - z| = |\chi(x, y, z) - z| - |x - \chi(x, y, z)|, \]  
\hspace{10cm} (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:

\[ E_{t+1}^i - E_t^i = -(S_t^i + S_{t+1}^i) \]  
\hspace{10cm} (77)

with energy current

\[ S_t^i := 1 - s_t^i - s_{t+1}^i. \]  
\hspace{10cm} (78)

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

Next, we devise the heat bath boundary condition by assigning Gibbs weights for the values of the virtual cells 0 and \( n + 1 \) (figure 8):

\[ P_0^L = \frac{1}{N_L} e^{-E_0/T_L}, \quad P_{n+1}^R = \frac{1}{N_R} e^{-E_{n+1}/T_R}. \]  
\hspace{10cm} (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

\[ \tilde{P}_L = \begin{pmatrix} 1/N_L & 1/N_L \\ e^{1/T_L}/N_L & e^{1/T_L}/N_L \\ 1 & 1 \end{pmatrix}, \]

\[ \tilde{P}_R = \begin{pmatrix} 1/N_R & 1/N_R \\ e^{-1/T_R}/N_R & e^{-1/T_R}/N_R \\ 1 & 1 \end{pmatrix}. \]  
\hspace{10cm} (80)
With (11), the boundary transition matrices are determined as follows:

\[
P^L = \begin{pmatrix}
\frac{1}{N_L} & \frac{1}{N_L} \\
\alpha & 1 - \beta \\
e^{1/T_x}/N_L & e^{1/T_x}/N_L \\
1 - \alpha & \beta
\end{pmatrix},
\]

\[
P^R = \begin{pmatrix}
\frac{1}{N_R} & \frac{1}{N_R} \\
\gamma & 1 - \delta \\
e^{-1/T_x}/N_R & e^{-1/T_x}/N_R \\
1 - \gamma & \delta
\end{pmatrix}.
\]

(81)

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

\[
q^L_1, q^L_2 \rightarrow 1/N_L, \quad 1 - q^R_1, q^R_2 \rightarrow e^{1/T_x}/N_L.
\]

\[
q^R_1, q^R_2 \rightarrow 1/N_R, \quad 1 - q^L_1, q^L_2 \rightarrow e^{-1/T_x}/N_R.
\]

The reduced NESS equations are immediately obtained:

\[
1 = (r_1 + r_2)/N_R,
\]

\[
r_2 = r_1[(1 - \gamma)r_3 + \delta r_8],
\]

\[
r_3 = r_1[\gamma r_2 + (1 - \delta)r_8],
\]

\[
r_4 = r_1(r_1 + r_2)e^{-1/T_x}/N_R,
\]

\[
r_5 = r_1[\gamma r_3 + (1 - \delta)r_4]/y_3,
\]

\[
r_6 = r_1[(1 - \gamma)r_3 + \delta r_4]/y_3,
\]

\[
r_7 = r_1(r_5 + r_6)/(y_1y_3N_R),
\]

\[
r_8 = r_1(r_5 + r_6)e^{-1/T_x}/(y_1y_3N_R).
\]

(82)

\[
r_1 = (1 + \lambda y_1)/N_L,
\]

\[
r_1 = (l_4 + l_6)/N_L,
\]

\[
r_1l_5 = y_3[\alpha + (1 - \beta)l_6],
\]

\[
r_1l_4 = y_3[\alpha l_2y_1 + (1 - \beta)l_5],
\]

\[
r_1l_5 = (1 + \lambda y_1)e^{1/T_x}/N_L,
\]

\[
r_1l_6 = (l_4 + l_6)e^{1/T_x}/N_L,
\]

\[
r_1l_7 = y_3[1 - \alpha + \beta l_6],
\]

\[
r_1l_8 = y_3[(1 - \alpha)l_3y_1 + \beta l_5],
\]

\[
r_7 = l_1/y_3.
\]

(83)

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

\[
\xi := \frac{1}{y_3} = \frac{1 - \lambda \mu + (1 - \mu)e^{1/T_x}}{[1 - \lambda \mu + (1 - \lambda)e^{-1/T_R}]^2} \left(\lambda e^{-1/T_R} + e^{1/T_R}(1 + e^{-1/T_R})\right),
\]

(85)

\[
\omega := y_1y_3 = \frac{1 - \lambda \mu + (1 - \lambda)e^{-1/T_R}}{[1 - \lambda \mu + (1 - \mu)e^{1/T_R}]^2} \left(\mu e^{1/T_R} + e^{-1/T_R}(1 + e^{1/T_R})\right).
\]

(86)
and the matrices \(L\) and \(R\) with parameters
\[
\begin{align*}
  r_1 &= \frac{1 - \lambda \mu + (1 - \lambda) e^{-1/T_L}}{1 - \lambda \mu + (1 - \mu) e^{1/T_L}}, \\
  r_2 &= \frac{(1 - \mu) \lambda e^{-1/T_R} + e^{1/T_L}(1 + e^{-1/T_R})}{1 - \lambda \mu + (1 - \mu) e^{1/T_L}}, \\
  r_3 &= r_1^2 \xi (e^{-1/T_R} + \mu), \\
  r_4 &= r_1 e^{-1/T_R}, \\
  r_5 &= r_1 \xi (\gamma r_3 + (1 - \delta) r_4), \\
  r_6 &= r_1 \xi [(1 - \gamma) r_3 + \delta r_4], \\
  r_7 &= r_1 \xi, \\
  r_8 &= r_1 \xi e^{-1/T_R}, \\
  l_3 &= \frac{e^{1/T_R} + \lambda}{r_1 \xi}, \\
  l_4 &= \frac{\alpha l_3 \xi \omega + (1 - \beta) e^{1/T_L}}{r_1 \xi}, \\
  l_5 &= l_6 = e^{1/T_L}, \\
  l_7 &= \frac{1 - \lambda}{r_1 \xi}, \\
  l_8 &= \frac{(1 - \alpha) l_3 \xi \omega + \beta e^{1/T_L}}{r_1 \xi},
\end{align*}
\]

where \(\lambda := \alpha - \beta e^{1/T_R}\) and \(\mu := \gamma - \delta e^{-1/T_R}\). It is noticeable that, unlike in the previous section, the exact solution is obtained without any conditions on the six parameters \(\alpha, \beta, \gamma, \delta, T_L,\) and \(T_R\). In the high temperature limit \(T_L = T_R = \infty\), the solution agrees with the Bernoulli boundary driving case \[9, 11\]. In addition, when we set \(\alpha = 1 - \beta, \gamma = 1 - \delta, 1/N_L = q_L^1,\) and \(1/N_R = q_R^1\), 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 the PSA is as follows:

\[
X = \begin{pmatrix}
  1 & 1 & 1 & 1 \\
  1 & 1 & e^{-2/T} & e^{-2/T} \\
  1 & 1 & e^{2/T} & e^{2/T} \\
  e^{2/T} & e^{2/T} & 1 & 1
\end{pmatrix},
\]

\(89\)
These can be written in the following form
\[
X_{s_1,s_2,s_3,s_4} = \exp \left[ 2s_1(s_2 - s_4)/T \right].
\]
\[
L_{s_1,s_2,s_3} = \exp \left[ s_1(1 - 2s_2)/T \right].
\]
\[
R_{s_n-2s_n-1} = \exp \left[ (2s_n-2s_{n-1} - 2s_{n-1}s_n - 1 + s_n)/T \right].
\]  
(91)

By substituting the three expressions into PSA (25) and rearranging them, we obtain
\[
p_s = \exp \left[ \left( s_1 + s_n - 1 + 2 \sum_{i=1}^{n-1} (-1)^i s_is_{i+1} \right)/T \right].
\]

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

3.4. Physical quantities in the NESS

3.4.1. Partition function. The exact solution (85)–(88) satisfies the eigenvalue equation
\[
IX = \tau_1 I, \quad Xr = \tau_1 r, \quad \Gamma X' = \tau_1 l', \quad X' r' = \tau_1 r',
\]  
(92)

where
\[
\tau_1 = \frac{[\lambda \mu - (1 + e^{1/T_1})(1 + e^{-1/T_1})]^2}{[1 - \lambda \mu + (1 - \mu)e^{1/T_1}][1 - \lambda \mu + (1 - \lambda)e^{-1/T_1}]}.
\]  
(93)

Then the partition functions are
\[
Z_n = \tau_1^{n/2-2} l \cdot r, \quad Z_n' = \tau_1^{n/2-2} l' \cdot r'.
\]  
(94)

From direct calculation, we find
\[
l \cdot r = l' \cdot r' = \frac{(1 + e^{1/T_1})(1 + e^{-1/T_1})}{1 - \lambda \mu + (1 - \mu)e^{1/T_1}} \left[ 1 - \lambda \mu + (\lambda + 2)e^{-1/T_1} + (\mu + 2)e^{1/T_1} + 3e^\Delta \beta \right]
\]  
(95)

where \( \Delta \beta = 1/T_1 - 1/T_n \), and then \( Z_n = Z_n' \).

3.4.2. Density. Substituting the exact solution into density definition (66), we obtain
\[
\rho_i = \frac{\lambda + 1)e^{-1/T_n} + (\mu + 1)e^{1/T_n} + 2e^\Delta \beta}{1 - \lambda \mu + (\lambda + 2)e^{-1/T_n} + (\mu + 2)e^{1/T_n} + 3e^\Delta \beta}
\]  
(96)

for \( 2 \leq i \leq n - 1 \). Thus, the density is uniform in this range, and the value is denoted as \( \rho \) in the following. For \( i = 1 \) and \( n \), \( \rho_i \) can take values different from \( \rho \); however, we do not show them because the equations are cumbersome. The temperature dependence of the bulk

\(^1\) Do not confuse inverse temperature difference \( \Delta \beta \) with the absorption rate \( \beta \).
density is illustrated in figure 9. Let us check some limiting behavior. For the emission limit \( \alpha, \gamma \to 1, \beta, \delta \to 0 (\lambda, \mu \to 1) \), the density takes the maximum value 2/3 regardless of temperature parameters. For the absorption limit \( \alpha, \gamma \to 0, \beta, \delta \to 1 (\lambda \to -e^{1/T_L}, \mu \to -e^{-1/T_R}) \), it becomes

\[
\rho = \frac{x}{2x + 1}, \quad x = e^{1/T_R} + e^{-1/T_L},
\]

and is in the range \( 0 < \rho \leq 1/2 \). \( \rho = 0 \) 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 the 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

\[
\rho \sim \frac{2}{4 - \lambda_0} + \frac{1 - \alpha}{(4 - \lambda_0)^2} \Delta \beta,
\]

and depends on the difference between the inverse temperatures.

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

\[
\rho_i = \frac{e^{1/T_L} + e^{-1/T_R} + 2e^{\Delta \beta}}{1 + 2e^{1/T_L} + 2e^{-1/T_R} + 3e^{\Delta \beta}},
\]

for \( 1 \leq i \leq n \) and in equilibrium \( T_L = T_R, \rho_i = 1/2 \).

3.4.3. Current. By substituting the exact solution into the definition of currents (69), we obtain

\[
J_R = \frac{\lambda e^{-1/T_R} + e^{1/T_R} + e^{\Delta \beta}}{1 - \lambda \mu + (\lambda + 2)e^{-1/T_R} + (\mu + 2)e^{1/T_R} + 3e^{\Delta \beta}},
J_L = \frac{\mu e^{1/T_L} + e^{-1/T_R} + e^{\Delta \beta}}{1 - \lambda \mu + (\lambda + 2)e^{1/T_R} + (\mu + 2)e^{1/T_L} + 3e^{\Delta \beta}}.
\]

The total current is \( J = J_R - J_L \). The behavior of the current is illustrated in figure 10. For the emission limit \( \lambda, \mu \to 1 \), 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

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

In the heat conduction limit, we have

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

It is remarkable that the current does not vanish in equilibrium \( (T_L = T_R = T) \) but has a finite value \( J = \frac{1}{2} \tanh \frac{1}{T} \).
3.4.4. 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 value of energy is given as
\[
\langle E_{2k} \rangle = 2\rho - 2J_R, \quad \langle E_{2k+1} \rangle = -2\rho + 2J_L.
\]
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
\[
E = \sum_{k=1}^{n/2-1} (\langle E_{2k} \rangle + \langle E_{2k+1} \rangle) = -(n - 2)J_L.
\]

Since the NESS vector does not depend on time, we can see immediately that the expectation value of energy flux is
\[
\langle S_i \rangle = 1 - 2\rho = \frac{1 - (\lambda + e^{1/T_L})(\mu + e^{-1/T_R})}{1 - \lambda \mu + (\lambda + 2)e^{-1/T_R} + (\mu + 2)e^{1/T_L} + 3e^{\Delta \beta}}.
\]
Thus, if the condition $(\lambda + e^{1/T_L})(\mu + e^{-1/T_R}) = 1$ or
\[
[\alpha + (1 - \beta)e^{1/T_L}][\gamma + (1 - \delta)e^{-1/T_R}] = 1
\]
holds, the energy current vanishes and the bulk density of 1 is 1/2. Under this condition, the matrices $X$, $R$, and $L$ are
\[
X = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & \phi^{-2} & \phi^{-2} \\ 1 & 1 & 1 & 1 \\ \phi^2 & \phi^2 & 1 & 1 \end{pmatrix}
\]
\[
L = \begin{pmatrix} 1 & 1 & 1 & 1 \\ \phi - \lambda & \phi - \lambda & 1 - \lambda & 1 - \lambda \end{pmatrix}.
\]
\[
R = \begin{pmatrix}
\phi^{-1} & 1 - \mu \\
\phi^{-1} & \phi^{-2}(1 - \mu \phi) \\
\phi^{-1} & 1 - \mu \\
\phi & 1 - \mu \phi
\end{pmatrix}
\]  \hspace{1cm} (107)

where \( \phi := \lambda + e^{1/T_L} \). Thus, we can represent the solution with only three parameters \( \phi, \lambda \), and \( \mu \). 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 \( \tau_1 \) are also simplified to

\[
l \cdot r = \frac{2N_LN_R(1 + \phi)}{\phi}, \quad \tau_1 = \frac{(1 + \phi)^2}{\phi}. \hspace{1cm} (108)
\]
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 state in this case is the same as the equilibrium one at temperature \( T = (\log \phi)^{-1} \) except for the density at the boundary cells. Such a state is illustrated in figure 11, where we see more lines downward to the right than 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 becomes
\[ \langle S_i \rangle \sim \frac{\lambda_0}{4 - \lambda_0} - \frac{2(1 - \alpha)}{(4 - \lambda_0)^2} \Delta \beta, \]  
\begin{equation} \tag{111} \end{equation}

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
\[ \langle S_i \rangle \sim (1 - \alpha)(T_L - T_R)/(8T_L T_R). \]

4. Discussion

We obtain two generalizations of Prosen and Mejía-Monasterio’s result on NESSs 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 zero or one with probability 1/2. We generalize this to \(\zeta\) and \(1 - \zeta\) for the left boundary and \(\eta\) and \(1 - \eta\) for the right boundary. The PSA is successfully applied to construct nonequilibrium steady states on the assumption (48) for the absorption and emission rates. 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 cannot verify it due to the complexity of the latter solution.

The other generalization 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 originates 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: the motion of particles, and the motion of energy. We think that the latter is more physical because it is based on a conservation law. In the case that both temperatures are equal and no absorption or emission occurs, equilibrium states are also naturally introduced at any temperature. Properties of energy transport are also studied under this boundary condition. The exact solution in the heat bath boundary case has been derived for any set of parameters without any additional conditions on absorption or emission rates. Moreover, this boundary condition includes Bernoulli boundary driving and 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 a uniform density of one in the bulk and ballistic transport. In the first solution, the current of particles is approximately proportional to $\gamma - \alpha$ when $\eta = \zeta$, and if the difference between $\alpha$ and $\gamma$ 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 the density profile, particle current, energy, and energy current in a variety of limiting cases. The particle current exists even in equilibrium states, where the energy current vanishes. This 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 a flat density profile and ballistic transport like RCA54, some show a nonzero density gradient near the boundaries and still ballistic transport, and 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. This is a future problem.

ORCID iDs

Atsuo Inoue  https://orcid.org/0000-0001-5530-1001
Shinji Takesue  https://orcid.org/0000-0002-7937-1298

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