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Ergodic Properties and Thermodynamic Behavior of Elementary Reversible Cellular Automata. I. Basic Properties

Shinji Takesue[1,2]

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This is the first part of a series devoted to the study of thermodynamic behavior of large dynamical systems with the use of a family of fully-discrete and conservative models named elementary reversible cellular automata (ERCAs). In this paper, basic properties such as conservation laws and phase space structure are investigated in preparation for the later studies. ERCAs are a family of one-dimensional reversible cellular automata having two Boolean variables on each site. Reflection and Boolean conjugation symmetries divide them into 88 equivalence classes. For each rule, additive conserved quantities written in a certain form are regarded as a kind of energy, if they exist. By the aid of the discreteness of the variables, every ERCA satisfies the Liouville theorem or the preservation of phase space volume. Thus, if an energy exists in the above sense, statistical mechanics of the model can formally be constructed. If a locally defined quantity is conserved, however, it prevents the realization of statistical mechanics. The existence of such a quantity is examined for each class and a number of rules which have at least one energy but no local conservation laws are selected as hopeful candidates for the realization of thermodynamic behavior. In addition, the phase space structure of ERCAs is analyzed by enumerating cycles exactly in the phase space for systems of comparatively small sizes. As a result, it is revealed that a finite ERCA is not ergodic, that is, a large number of orbits coexist on an energy surface. It is argued that this fact does not necessarily mean the failure of thermodynamic behavior on the basis of an analogy with the ergodic nature of infinite systems.

KEY WORDS: Reversible cellular automaton; statistical mechanics; thermodynamic behavior; ergodic properties; additive invariant; phase space structure.

[1] Research Institute for Fundamental Physics, Kyoto University, Kyoto 606, Japan.
[2] Present address: Department of Physics, Faculty of Science, Gakushuin University, Toshima-ku, Tokyo 171, Japan.

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1. INTRODUCTION

Although statistical mechanics has more than a century of successful history since the age of Boltzmann, its dynamical foundation has not been established as yet. Even the use of the Gibbs ensemble, which plays the central role in statistical mechanics, is postulated as an Ansatz and has not been derived from first principles, that is, microscopic dynamics of the system.

It is ergodic theory that should link the dynamics and statistical mechanics. Ergodic theory has been developed considerably by mathematicians and has produced a variety of concepts and theorems. For example, a hierarchy of ergodic-theoretic properties has been found: Bernoulli > K-property > mixing > ergodicity, where the inequalities represent the strength of these properties; every Bernoulli system is a K-system, every K-system is mixing, and every mixing system is ergodic.[1] Of these properties, ergodicity justifies the use of microcanonical ensemble and mixing implies a kind of relaxation property. As the Kolmogolov–Arnol'd–Moser theorem[2] has revealed, however, even ergodicity is not generic for mechanical systems with a finite number of degrees of freedom. On the other hand, the Bernoulli property, the top of the hierarchy, is achieved by such simple *infinite* systems as the noninteracting ideal gas,[3,4] the complete harmonic crystal,[5] and the one-dimensional hard rod system.[3] Although this looks strange, it only means that local perturbations can escape to infinity in such systems. It is, therefore, not very relevant to physics; for example, these infinite systems show relaxation only in some physically limited situations. Thus, the study of asymptotic behavior of large systems is needed.

Reversible cellular automata provide clear examples to investigate the problem.[6] A cellular automaton is a dynamical system composed of discrete variables on a discrete space-time.[7] The states of all the variables are synchronously updated at every time step according to a deterministic rule which is locally defined and uniform in space. If a cellular automaton is reversible or bijective, that is, if each configuration has a unique predecessor, it automatically satisfies the Liouville theorem or the preservation of phase space volume by virtue of the discreteness of the variables. Consequently, the statistical mechanics of the model can be constructed, provided that it has a global conserved quantity which can be regarded as a kind of energy. Examples of such quantities have been shown by Pomeau[8] for a particular type of reversible cellular automata having "voting" rules. Other examples will be shown later in this paper. In such cases, one can compare the results of the statistical mechanics (ensemble averages) with those of dynamics (time averages). This is a test of ergodicity in the physical sense.

Equilibrium properties can be investigated in this manner. Nonequilibrium behavior is capable of being studied in a similar manner within the scope of linear response theory. In any case, numerical simulations are always possible.

The relation between dynamics and statistical mechanics is usually studied in relation to Hamiltonian systems.[9] The formalism of statistical mechanics only demands the preservation of phase space volume and energy conservation. The symplectic condition for dynamics is not necessary as concerns the problem of the foundation of statistical mechanics. In this sense, the reversible cellular automata satisfy the conditions for statistical mechanics to be discussed. Furthermore, the contrast between Hamiltonian systems and the reversible cellular automata may elucidate some role of the symplectic condition which is not appreciated from the study of only Hamiltonian systems.

Recent applications of cellular automata as a tool of numerical simulations are also relevant to the present problem. The features of cellular automata are strikingly suitable for execution by digital computers, especially with the help of massively parallel processing architecture. In particular, cellular automata are fast and free from roundoff errors. Thus, large-scale simulations may comparatively easily be carried out by utilizing cellular automata. Taking advantage of this, a number of deterministic Ising dynamics, such as Creutz's model,[10] Q2R,[11–13] and their variations,[14,15] have been devised as an alternative to Monte Carlo calculations, and lattice-gas automata for simulations of the Navier–Stokes equation.[16] Both of these are reversible cellular automata constructed so as to satisfy necessary symmetries and conservation laws at the microscopic level. They are no more than crude approximations or artifacts on this microscopic level. Nevertheless, their macroscopic nature is expected to be physical, if they show standard thermodynamic behavior[17] with respect to such points as equilibrium statistics described by a canonical ensemble, relaxation to equilibrium, local equilibrium in a nonequilibrium steady state, and the Kubo formula for transport coefficients. Although successful simulation results have been reported, it has not been clarified for what conditions the thermodynamic behavior is realized. This is just the problem which I will consider.

One great advantage of a study of cellular automata lies in the fact that the number of possible rules is finite if the shape of the lattice, the number of distinct values for variables on each site, and the interaction range are specified. Thus, one can thoroughly investigate *all* the models that belong to a fairly general set and classify them according to some physical or mathematical properties. The classification thus obtained will be useful for the construction of a general theory. This follows the

approach taken by Wolfram.[18] In his pioneering work, he studied a family of one-dimensional cellular automata and classified them into four classes according to qualitative differences of spatiotemporal patterns generated. In the present series of papers, I present a family of one-dimensional *reversible* cellular automata called elementary reversible cellular automata (ERCAs),[6] which can be seen as a second-order variant of Wolfram's models. Energy is introduced for some ERCAs, which then are classified with respect to the degree of realization of thermodynamic behavior. In the course of the study, various stages of thermodynamic behavior will be observed in a number of models. Thus, it is concluded that ERCAs serve as a minimal model for the study of the thermodynamic behavior of large dynamical systems.

This paper is the first part of a series which concerns basic properties of ERCAs such as conservation laws and phase space structure. On the basis of the knowledge obtained here, the realization of equilibrium and nonequilibrium thermodynamic behavior will be examined in the subsequent papers. In Section 2, the models are defined and classified according to symmetry properties. In Section 3, ERCAs are searched for additive conserved quantities in a certain form, which are regarded as energy if they exist. In Section 4, the existence of local conservation laws, which prevent the realization of the statistical mechanics, is examined for each rule. As a result of Sections 3 and 4, a subset of rules which have additive conserved quantities but no local conservation laws is selected for later use in the subsequent papers. Phase space structure of ERCAs is investigated in Section 5, where it is revealed that a large number of orbits coexist on an energy surface in a finite ERCA. This fact does not immediately mean the failure of thermodynamic behavior, however. Section 6 is devoted to a summary and discussion.

2. MODELS AND SYMMETRIES

ERCAs are a family of one-dimensional reversible (bijective) cellular automata where each site i has two Boolean variables σ_i^t and $\hat{\sigma}_i^t$ evolving according to a rule of the following form[6]:

$$\sigma_i^{t+1} = f(\sigma_{i-1}^t, \sigma_i^t, \sigma_{i+1}^t) \text{ XOR } \hat{\sigma}_i^t \tag{2.1}$$

$$\hat{\sigma}_i^{t+1} = \sigma_i^t \tag{2.2}$$

where integer t denotes discrete time, f is a Boolean function of three variables, and XOR means the "exclusive OR" operation. All the Boolean variables and functions take values in the set of $\{0, 1\}$, which are treated

as integers with the usual arithmetic. For such variables σ and μ, σ XOR $\mu = \sigma + \mu - 2\sigma\mu$ in the usual representation. Equations (2.1) and (2.2) have another representation of the second-order difference form:

$$\sigma_i^{t+1} = f(\sigma_{i-1}^t, \sigma_i^t, \sigma_{i+1}^t) \text{ XOR } \sigma_i^{t-1} \tag{2.3}$$

From this equation the time-reversal evolution is explicitly obtained as

$$\sigma_i^{t-1} = f(\sigma_{i-1}^t, \sigma_i^t, \sigma_{i+1}^t) \text{ XOR } \sigma_i^{t+1} \tag{2.4}$$

which has just the same form as Eq. (2.3). That is, ERCAs are not only reversible, but also time-reversal invariant, as are classical mechanical systems.

The use of the term "elementary" (the E of ERCAs) is after Wolfram. He studied one-dimensional cellular automata having the following form of time evolution rules[18]:

$$\sigma_i^{t+1} = f(\sigma_{i-1}^t, \sigma_i^t, \sigma_{i+1}^t) \tag{2.5}$$

and referred to them as "elementary rules." ERCAs are their second-order generalizations. In general, when a first-order rule is given as

$$\sigma_i^{t+1} = f(\{\sigma_j^t\}_{j \in U_i}) \tag{2.6}$$

with arbitrary variables $\{\sigma_i^t\}$, arbitrary neighborhood U_i of site i, and an arbitrary function f, one can construct a time-reversal invariant second-order rule as

$$\sigma_i^{t+1} = f(\{\sigma_j^t\}_{j \in U_i}) - \sigma_i^{t-1} \tag{2.7}$$

This is called a Fredkin construction.[11] Though they have not been referred to by this name, ERCAs are mentioned in a number of papers.[7,19] However, almost all of their descriptions are fragmentary. The present paper is the first attempt at their systematic research.

ERCAs contain as many rules as there are possible Boolean functions of three variables, namely $2^{2^3} = 256$ rules. An ERCA specified by such a Boolean function f is termed fR or the number $\sum_{\mu,\nu,\kappa} 2^{4\mu+2\nu+\kappa} f(\mu, \nu, \kappa)$ with an R standing for "reversible" appended to it. This coding for the Boolean function is the same as Wolfram's. For example, the rule with the function $f(\mu, \nu, \kappa) = \mu$ XOR κ is called 90R.

As is known from the above definition, $\hat{\sigma}_i^t$ is introduced only to make the dynamics be second order. It never is the variable conjugate to σ_i^t as is the momentum to the position in Hamiltonian dynamical systems. In fact, it is impossible to introduce the symplectic condition for ERCAs, since it

is based on the differential structure. Of course, some analogies will survive as a benefit of the reversibility and in some cases the use of these analogies will be an aid for understanding.

Consider a system which is an N-site chain with the cyclic boundary condition imposed to keep reversibility. The set of values for the Boolean variables at time t is denoted by

$$x^t = (\boldsymbol{\sigma}^t, \hat{\boldsymbol{\sigma}}^t) \tag{2.8}$$

where the Boolean N-vectors $\boldsymbol{\sigma}^t$ and $\hat{\boldsymbol{\sigma}}^t$ are given by

$$\boldsymbol{\sigma}^t = (\sigma_1^t, ..., \sigma_N^t) \tag{2.9}$$

$$\hat{\boldsymbol{\sigma}}^t = (\hat{\sigma}_1^t, ..., \hat{\sigma}_N^t) \tag{2.10}$$

In this vector notation an ERCA dynamics which is the set of local rules (2.1) is written as

$$\boldsymbol{\sigma}^{t+1} = \mathbf{f}(\boldsymbol{\sigma}^t) \,\mathrm{XOR}\, \hat{\boldsymbol{\sigma}}^t \tag{2.11}$$

where $\mathbf{f}(\boldsymbol{\sigma})$ is an N-vector Boolean function given by

$$\mathbf{f}(\boldsymbol{\sigma}) = (f(\sigma_N, \sigma_1, \sigma_2), f(\sigma_1, \sigma_2, \sigma_3), ..., f(\sigma_{N-1}, \sigma_N, \sigma_1)) \tag{2.12}$$

and for Boolean N-vectors $\boldsymbol{\alpha} = (\alpha_i)$ and $\boldsymbol{\beta} = (\beta_i)$, $\boldsymbol{\alpha}\,\mathrm{XOR}\,\boldsymbol{\beta}$ is defined by $(\alpha_i \,\mathrm{XOR}\, \beta_i)$.

The phase space for such an ERCA is the set of possible configurations for the dynamical variables,

$$\begin{aligned} \Omega_N &= \{(\boldsymbol{\sigma}, \hat{\boldsymbol{\sigma}}) = (\sigma_1, ..., \sigma_N, \hat{\sigma}_1, ..., \hat{\sigma}_N)\} \\ &\cong \{0, 1\}^{2N} \end{aligned} \tag{2.13}$$

which therefore consists of 4^N points. The ERCA dynamics is a bijective mapping of the phase space Ω_N onto itself. Hence, the phase space volume is preserved in ERCAs. This is due to the discreteness of the variables. An orbit of an ERCA is a set of points, $\{x^t = (\boldsymbol{\sigma}^t, \hat{\boldsymbol{\sigma}}^t)\}_{-\infty < t < \infty}$. Because $\hat{\boldsymbol{\sigma}}^t = \boldsymbol{\sigma}^{t-1}$, the orbit can be completely represented by the set $\{\boldsymbol{\sigma}^t\}_{-\infty < t < \infty}$ only. Since the number of points in the phase space is finite and the time evolution is reversible, any orbit is a cycle or a periodic orbit. This cycle corresponds to the Poincaré recurrence. The distribution of cycle lengths is investigated in Section 5.

Two symmetries lead to isomorphisms between rules. Orbits in corresponding rules, as well as the rules themselves, can be one-to-one transformed into each other by the symmetry operations. Such rules are grouped into an equivalence class and can be seen as identical, because

they have the same structure of the phase space. One such symmetry is reflection, and the other is Boolean conjugation.[11]

Reflection means left–right inversion. Rule gR with the Boolean function g defined by

$$g(\mu, \nu, \kappa) = f(\kappa, \nu, \mu) \tag{2.14}$$

is called the reflection of rule fR. An orbit in the reflection, $\{\boldsymbol{\phi}^t\}$, can be made from an orbit $\{\boldsymbol{\sigma}^t\}$ in rule fR by the transformation

$$\phi_i^t = \sigma_{N-i}^t \tag{2.15}$$

Boolean conjugation is exchange of the roles of 0 and 1. Thus, the transformation between orbits $\{\boldsymbol{\psi}^t\}$ and $\{\boldsymbol{\sigma}^t\}$ in the corresponding rules must be given by

$$\psi_i^t = 1 - \sigma_i^t \tag{2.16}$$

This is achieved by the transformation of Boolean function

$$h(\mu, \nu, \kappa) = f(1-\mu, 1-\nu, 1-\kappa) \tag{2.17}$$

and the rule hR is called the conjugate of rule fR. It should be noted that this operation is different from the Boolean conjugation for Wolfram's elementary cellular automata. In the latter case, the following is the transformation leading to Eq. (2.16)[3]:

$$h(\mu, \nu, \kappa) = 1 - f(1-\mu, 1-\nu, 1-\kappa) \tag{2.18}$$

This is the combination of the transformation (2.17) and one, called the complement by Vichniac,[11] for reversible rules of Fredkin-construction type whose transformation is written as

$$h(\mu, \nu, \kappa) = 1 - f(\mu, \nu, \kappa) \tag{2.19}$$

The complement does not generally lead to isomorphisms, but yields a number of interesting relations between orbits discussed in Appendix A.

As is shown in Table I, the reflection and the Boolean conjugation symmetries divide ERCAs into 88 equivalence classes. Each class is denoted by the minimal numbered representative in a bracket as, say, [0R]. Except for the case particularly stated, henceforth I treat only the minimal numbered representatives, which are shown in the first column in Table I.

[3] Due to this difference, Wolfram's elementary cellular automata have a classification of rule numbers different from the present one. Accordingly, a Wolfram rule and its second-order variant of ERCA do not necessarily have similar characteristics, though they are denoted by a common number.

Table I. 88 Equivalence Classes[a]

Rule	Conj	Refl	CR	Comp	Rule	Conj	Refl	CR	Comp
0R	0R	0R	0R	[255R]	59R	220R	115R	206R	[35R]
1R	128R	1R	128R	[127R]	60R	60R	102R	102R	[153R]
2R	64R	16R	8R	[191R]	61R	188R	103R	230R	[25R]
3R	192R	17R	136R	[63R]	62R	124R	118R	110R	[131R]
4R	32R	4R	32R	[223R]	63R	252R	119R	238R	[3R]
5R	160R	5R	160R	[95R]	73R	146R	73R	146R	[109R]
6R	96R	20R	40R	[159R]	75R	210R	89R	154R	[45R]
7R	224R	21R	168R	[31R]	77R	178R	77R	178R	[77R]
9R	144R	65R	130R	[111R]	79R	242R	93R	186R	[13R]
10R	80R	80R	10R	[175R]	90R	90R	90R	90R	[165R]
11R	208R	81R	138R	[47R]	91R	218R	91R	218R	[37R]
12R	48R	68R	34R	[187R]	94R	122R	94R	122R	[133R]
13R	176R	69R	162R	[79R]	95R	250R	95R	250R	[5R]
14R	112R	84R	42R	[143R]	105R	150R	105R	150R	[105R]
15R	240R	85R	170R	[15R]	107R	214R	121R	158R	[41R]
18R	72R	18R	72R	[183R]	109R	182R	109R	182R	[73R]
19R	200R	19R	200R	[55R]	111R	246R	125R	190R	[9R]
22R	104R	22R	104R	[151R]	123R	222R	123R	222R	[33R]
23R	232R	23R	232R	[23R]	126R	126R	126R	126R	[129R]
24R	24R	66R	66R	[189R]	127R	254R	127R	254R	[1R]
25R	152R	67R	194R	[61R]	129R	129R	129R	129R	[126R]
26R	88R	82R	74R	[167R]	131R	193R	145R	137R	[62R]
27R	216R	83R	202R	[39R]	133R	161R	133R	161R	[94R]
28R	56R	70R	98R	[157R]	135R	225R	149R	169R	[30R]
29R	184R	71R	226R	[29R]	139R	209R	209R	139R	[46R]
30R	120R	86R	106R	[135R]	141R	177R	197R	163R	[58R]
31R	248R	87R	234R	[7R]	143R	241R	213R	171R	[14R]
33R	132R	33R	132R	[123R]	147R	201R	147R	201R	[54R]
35R	196R	49R	140R	[59R]	151R	233R	151R	233R	[22R]
36R	36R	36R	36R	[219R]	153R	153R	195R	195R	[60R]
37R	164R	37R	164R	[91R]	155R	217R	211R	203R	[38R]
38R	100R	52R	44R	[155R]	157R	185R	199R	227R	[28R]
39R	228R	53R	172R	[27R]	159R	249R	215R	235R	[6R]
41R	148R	97R	134R	[107R]	165R	165R	165R	165R	[90R]
43R	212R	113R	142R	[43R]	167R	229R	181R	173R	[26R]
45R	180R	101R	166R	[75R]	175R	245R	245R	175R	[10R]
46R	116R	116R	46R	[139R]	179R	205R	179R	205R	[50R]
47R	244R	117R	174R	[11R]	183R	237R	183R	237R	[18R]
50R	76R	50R	76R	[179R]	187R	221R	243R	207R	[12R]
51R	204R	51R	204R	[51R]	189R	189R	231R	231R	[24R]
54R	108R	54R	108R	[147R]	191R	253R	247R	239R	[2R]
55R	236R	55R	236R	[19R]	219R	219R	219R	219R	[36R]
57R	156R	99R	198R	[57R]	223R	251R	223R	251R	[4R]
58R	92R	114R	78R	[141R]	255R	255R	255R	255R	[0R]

[a] The first column only contains the minimal numbered representatives of the classes. "Conj" denotes the Boolean conjugation, "Refl" denotes the reflection, and "CR" denotes the combined operation of the Boolean conjugation and the reflection. These four constitute a class. The last column shows its complement class.

3. ADDITIVE CONSERVED QUANTITIES

As stated in Section 1, energy must be introduced to construct the statistical mechanics of ERCAs. However, an ERCA is defined as a time-evolution rule and does not have an *a priori* Hamiltonian. Hence, I define an energy as an additive conserved quantity. The additivity means that the energy must be written as a sum of local quantities. I here choose as candidates for energy the following form of additive quantities:

$$\Phi(x) = \sum_i F(\sigma_i, \sigma_{i+1}, \hat{\sigma}_i, \hat{\sigma}_{i+1}) \tag{3.1}$$

where $x = (\boldsymbol{\sigma}, \hat{\boldsymbol{\sigma}})$ denotes a point in the phase space Ω_N. The constraint that the function F depends upon two adjacent sites is made only for simplicity, but it equips the quantity Φ with the picture that bond $(i, i+1)$ has an energy

$$F^t_{i,i+1} = F(\sigma^t_i, \sigma^t_{i+1}, \hat{\sigma}^t_i, \hat{\sigma}^t_{i+1}) \tag{3.2}$$

at time t. If such a quantity exists, the partition function Z is given by

$$\begin{aligned} Z &= \sum_{x \in \Omega_N} \exp[-\beta \Phi(x)] \\ &= \sum_{\sigma_1, \hat{\sigma}_1, \ldots, \sigma_N, \hat{\sigma}_N} \cdots \sum \prod_i \exp[-\beta F(\sigma_i, \sigma_{i+1}, \hat{\sigma}_i, \hat{\sigma}_{i+1})] \end{aligned} \tag{3.3}$$

which has a form similar to the one-dimensional Ising system and therefore can be evaluated with the method of transfer matrix. Thermodynamic quantities are calculated through the partition function or the transfer matrix.

Here, what is to be solved first is to find F such that Φ be an invariant for given f. Now I examine this for each of the 88 representatives obtained in Section 2.

First consider a general form of the function F. Because this function is of four Boolean variables, its arguments take $2^4 = 16$ possible values. Thus, 16 parameters are needed to determine such a function in general. In the present case, however, the number can be reduced by utilizing the facts that the zero value of an energy can be arbitrarily chosen and that F is a function to be summed over sites. The former permits one to put $F(0, 0, 0, 0) = 0$. The latter implies that a value of $\Phi(x)$ is determined by only the set of numbers, each representing the frequency of a two-site configuration appearing in the phase point x. These numbers satisfy the following sum rules: denoting by $\pi(a, b, c, d \mid x)$ the number of sites i such that $(\sigma_i, \sigma_{i+1}, \hat{\sigma}_i, \hat{\sigma}_{i+1}) = (a, b, c, d)$ in $x = (\boldsymbol{\sigma}, \hat{\boldsymbol{\sigma}})$, one has

$$\sum_{a,b} \pi(a, 0, b, 0 \mid x) = \sum_{a,b} \pi(0, a, 0, b \mid x) \tag{3.4a}$$

$$\sum_{a,b} \pi(a, 0, b, 1 \mid x) = \sum_{a,b} \pi(0, a, 1, b \mid x) \tag{3.4b}$$

$$\sum_{a,b} \pi(a, 1, b, 0 \mid x) = \sum_{a,b} \pi(1, a, 0, b \mid x) \tag{3.4c}$$

$$\sum_{a,b} \pi(a, 1, b, 1 \mid x) = \sum_{a,b} \pi(1, a, 1, b \mid x) \tag{3.4d}$$

Only three of these are independent. By the utilization of the above two facts, the number of the necessary parameters is reduced by four. A general form of the function F is written as

$$\begin{aligned} F(\alpha, \beta, \hat{\alpha}, \hat{\beta}) = {} & b_1(\alpha+\beta) + b_2(\hat{\alpha}+\hat{\beta}) + b_3\alpha\beta + b_4\hat{\alpha}\hat{\beta} + b_5(\alpha\hat{\alpha}+\beta\hat{\beta}) + b_6\alpha\hat{\beta} \\ & + b_7\beta\hat{\alpha} + b_8\alpha\beta\hat{\alpha} + b_9\alpha\beta\hat{\beta} + b_{10}\alpha\hat{\alpha}\hat{\beta} + b_{11}\beta\hat{\alpha}\hat{\beta} + b_{12}\alpha\beta\hat{\alpha}\hat{\beta} \end{aligned} \tag{3.5}$$

with the use of 12 parameters $\{b_i\}$.

Substituting the above form into the equation $\Phi^{t+1} = \Phi^t$ and representing the variables at time $t+1$ by those at time t with the use of Eqs. (2.1) and (2.2), I obtain the following set of equations for $\{b_i\}$ as the necessary and sufficient condition that Φ be conserved:

$$b_1 = b_2 \tag{3.6a}$$

$$b_3 = b_4 \tag{3.6b}$$

$$b_8 + b_9 = b_{10} + b_{11} \tag{3.6c}$$

$$\begin{aligned} & 2(b_3 + b_8\sigma_i + b_9\sigma_{i+1} + b_{12}\sigma_i\sigma_{i+1})(f_i - f_{i+1})^2 \\ & \quad = (b_8 - b_{10})(\sigma_i - \sigma_{i+1}) \end{aligned} \tag{3.6d}$$

$$\begin{aligned} & \{4b_1 + 2b_3 + (2b_7 + b_8)\,\sigma_{i-1} + (4b_5 + b_8 + b_9)\,\sigma_i + (2b_6 + b_9)\,\sigma_{i+1} \\ & \qquad + (2b_{10} + b_{12})\,\sigma_{i-1}\sigma_i\}\, f_i \\ & \quad = [b_7 - b_6 + (b_8 - b_{10})(\sigma_i + 1/2)](\sigma_{i-1} - \sigma_{i+1}) \end{aligned} \tag{3.6e}$$

where $f_i = f(\sigma_{i-1}, \sigma_i, \sigma_{i+1})$ and the last two equations have to hold for arbitrary values of $(\sigma_{i-1}, \sigma_i, \sigma_{i+1}, \sigma_{i+2})$. The derivation of these equations is explained in detail in Appendix B.

These equations always have the trivial solution that all $b_i = 0$. Other solutions are, if they exist, determined up to the ratio among parameter

Table II. Additive Invariants for the 88 Rules[a]

Rule	$b_1 = b_2$	$b_3 = b_4$	b_5	b_6	b_7	b_8	b_9	b_{10}	b_{11}	b_{12}
0R	1									
		1								
			1							
				1	1					
						1		1		
							1		1	
										1
1R			1							
				1	1					
						1		1		
							1		1	
										1
2R	1			−2	−2					
			1							
						1		1		
										1
3R			1							
						1		1		
										1
4R	1		−1							
		1				−1	−1	−1	−1	
				1	1					
										1
5R				1	1					
										1
6R	1		−1	−2	−2					
										1
7R										1
9R			1	−2	−2					
			1			−2		−2		2
10R	1			−2	−2					
			1			−2		−2		2
11R			1			−2		−2		2
12R	1		−1							
		1		1	1	−1	−1	−1	−1	1

[a] Nontrivial solutions $\{b_t\}$ for (3.6a)–(3.6e) are shown. Blank means that the value is zero. Rules absent from this table do not have any additive invariants of the form (3.1).

Table II. *(Continued)*

Rule	$b_1 = b_2$	$b_3 = b_4$	b_5	b_6	b_7	b_8	b_9	b_{10}	b_{11}	b_{12}
18R	1			−2	−2					
		1								
										1
19R	1	−2		−1	−1	2	2	2	2	
			1							
										1
22R	1		−1	−2	−2					
										1
23R	1	−2	−1	−1	−1	2	2	2	2	
										1
24R	1			−2	−2					
26R	1			−2	−2					
27R	2	−4	−3	−2	−2	4	4	4	4	−4
33R			1							
										1
35R			1							
										1
36R	1		−1	−1	−1					
		1				−1	−1	−1	−1	
										1
37R										1
38R										1
39R										1
46R	1						−4		−4	4
50R			1							
				3	−3	2	−2	−2	2	
										1
51R	1		−2	−1	−1	2	2	2	2	
		1								
				3	−3	2	−2	−2	2	
										1
54R										1

Table II. *(Continued)*

Rule	$b_1 = b_2$	$b_3 = b_4$	b_5	b_6	b_7	b_8	b_9	b_{10}	b_{11}	b_{12}
55R	1	−2	−1	−1	−1	2	2	2	2	1
59R	2	−4	−3	−2	−2	4	4	4	4	−4
73R			1	−2	−2					
77R				1	−1	2	−2	−2	2	
90R	1			−2 1	−2 −1					
91R	2	−4	−3	−2 1	−2 −1	4	4	4	4	−4
94R				1	−1					
95R				1	−1					
123R	2	−4	−3	−2 1	−2 −1	4	4	4	4	−4
126R			1	1 1	1 −1	−2	−2	−2	−2	4
127R			1	1 1	1 −1	−2	−2	−2	−2	4
129R			1 1	 1	 1	−2 −1	 −2 −1	−2 −1	 −2 −1	2 2 2
131R			1			−2		−2		2
139R			1			−2		−2		2
179R	1	−2	−2	−1 3	−1 −3	2 2	2 −2	2 −2	2 2	
219R	1	−2	−1	−1 1	−1 −1	2	2	2	2	−4
223R	1	−2	−1	−1 1	−1 −1	2	2	2	2	−4
255R	1	−2	1	1 1	1 −1	−2	−2	−2	−2	4

values. All nontrivial solutions for the 88 representatives are shown in Table II, where absolute values for $\{b_i\}$ are chosen as simple as possible. When a representative of a class has such a quantity, other rules in the same class also conserve its variants transformed according to the symmetry property of the rules.

Table II teaches one that an ERCA may have more than one additive conserved quantity and that conversely more than one rule may have a common invariant Φ. Moreover, a number of rules do not have any additive conserved quantities of the form (3.1). These facts reflect that this type of conserved quantity does not govern the dynamics of ERCAs as do the Hamiltonians in mechanics.

It is found that a certain additive conserved quantity Φ is not invariant, but is periodically varying in time for a number of rules. This is a consequence of the complement symmetry mentioned in Section 2. Details are shown in Appendix A.

Additive invariants in cellular automata were first studied by Pomeau.[8,20] Applied to the present case, his result says that if the function $f(\mu, \nu, \kappa)$ takes unity only when $\mu - a\nu + \kappa = q$ with constants a and q, the additive quantity denoted by $(b_1, b_2, b_5, b_6, b_7) = (q, q, a, -2, -2)$ (others not mentioned are zeros, which convention is used henceforth) is invariant. In Table I, rules 90R ($a=0$, $q=1$), 73R ($a=1$, $q=0$), 36R ($a=-2$, $q=2$), and 22R ($a=-1$, $q=1$) are such cases. This kind of quantity is also conserved in rules where f does not necessarily take unity if $\mu - a\nu + \kappa = q$. For example, rules 26R, 24R, 18R, 10R, 4R, 2R, and 0R have the invariant $(b_1, b_2, b_6, b_7) = (1, 1, -2, -2)$ in common with 90R. Another case also has a similar sequence of rules.

Table I contains more than Pomeau's type. For example, quantities with nonzero parameters other than $b_1 = b_2$, b_5, b_6, and b_7 do not belong to Pomeau's type. Such additive conserved quantities are found in the present paper for the first time. These include antisymmetric [e.g., $(b_6, b_7) = (1, -1)$ for rules 90R, 91R, 94R, etc.] or asymmetric [e.g., $(b_1, b_2, b_9, b_{11}, b_{12}) = (1, 1, -4, -4, 4)$ for rule 46R] ones with respect to the reflection or the exchange of variables between σ's and $\hat{\sigma}$'s, while Pomeau-type invariants are symmetric for both operations. "Energy" does not usually have such a symmetry property. Though another name might better suit such quantities, I call them energy without distinction for simplicity.

If a nontrivial solution exists for Eqs. (3.6a)–(3.6e), the equation of continuity is constructed at the same time. That is, flow can be defined so that the temporal variation of bond energy is written as the difference between incoming and outgoing flows

$$F^{t+1}_{i,i+1} = F^{t}_{i,i+1} + J^{t}_{i} - J^{t}_{i+1} \tag{3.7}$$

where J_i^t is the flow at site i at time t given by the following function:

$$\begin{aligned} J_i^t &= J(\sigma_{i-1}^t, \sigma_i^t, \sigma_{i+1}^t, \hat{\sigma}_i^t) \\ &= 1/4\{2f_i^t(1-2\hat{\sigma}_i^t)[2b_1 + b_3 + (2b_5 + b_8)\,\sigma_i^t \\ &\quad + (2b_6 + b_9)\,\sigma_{i+1}^t + (2b_{10} + b_{12})\,\sigma_i^t\sigma_{i+1}^t] \\ &\quad + 2(b_6 - b_7)(2\sigma_{i+1}^t\hat{\sigma}_i^t - \sigma_i^t - \sigma_{i+1}^t) \\ &\quad + (b_8 - b_{10})[2\sigma_i^t\hat{\sigma}_i^t + \sigma_{i+1}^t(1+2\sigma_i^t)(1-\hat{\sigma}_i^t)]\} \\ &\quad + \text{const} \end{aligned} \tag{3.8}$$

where $f_i^t = f(\sigma_{i-1}^t, \sigma_i^t, \sigma_{i+1}^t)$. It is easily ascertained that Eq. (3.8) satisfies Eq. (3.7) with the help of Eqs. (3.6). Note that Eq. (3.7) defines J_i^t up to an additional constant, which has to be determined by another condition, for example, that the ensemble average $\langle J_i \rangle = 0$ in equilibrium states.

I address a number of remarks at the end of the present section. First, the quantity Φ is not affected by adding to the function F the terms

$$c_1(\sigma_i - \sigma_{i+1}) + c_2(\hat{\sigma}_i - \hat{\sigma}_{i+1}) + c_3(\sigma_i\hat{\sigma}_i - \sigma_{i+1}\hat{\sigma}_{i+1}) \tag{3.9}$$

where c_1, c_2, and c_3 are arbitrary constants. Correspondingly, the flow is modified by the additional terms

$$(c_2 - c_1)(\sigma_i - \hat{\sigma}_i) + (c_1 + c_3\sigma_i)(1-2\hat{\sigma}_i)f_i \tag{3.10}$$

This arbitrariness has been already used in the argument for the number of parameters necessary for identifying F.

Second, though I restrict the function F to be of variables on two adjacent sites, there is a possibility that a sum of local functions of more variables is conserved. Indeed, the fact that $\Phi' = \sum_i\{(\sigma_i^t - \hat{\sigma}_{i+1}^t)^2 + (\hat{\sigma}_i^t - \sigma_{i+1}^t)^2\}$ has period two in a number of rules means that such rules conserve $\Phi^t + \Phi^{t+1}$ and $|\Phi^{t+1} - \Phi^t|$, which are represented using variables at time t as

$$\Phi^t + \Phi^{t+1} = 2\sum_i\{(1-2\hat{\sigma}_i^t)(1-\sigma_{i-1}^t - \sigma_{i+1}^t)(f_i^t - 1) + 1\} \tag{3.11}$$

$$|\Phi^{t+1} - \Phi^t| = 2\left|\sum_i (1-2\hat{\sigma}_i^t)(1-\sigma_{i+1}^t - \sigma_{i-1}^t)f_i^t\right| \tag{3.12}$$

Each term in the above summations is a function of variables on three adjacent sites. In addition, the existence of local conservation laws involving more than two sites, discussed in the next section, implies that this kind of additive conserved quantity may be commonly seen. Since

thermodynamic behavior should be strongly affected by the existence of such quantities, it is worthwhile to seek them. When many variables are involved, however, straightforward calculation as in the present section becomes a hard task. Thus, this problem is left for the future.

Finally, in order for the summation to be conserved, the summand need not be homogeneous in space. It may alternate on successive bonds. In peripheral rules[18] where $f(\mu, \nu, \kappa)$ does not depend on ν, an orbit is decomposed into two independent parts in the (i, t) plane like the black and white of the checkerboard. Thus, an additive invariant, if any, can be defined on each color of the checkerboard and the summand necessarily is alternate. The peripheral rules belong to the classes [0R], [5R], [10R], [15R], [90R], [95R], [165R], [175R], and [255R].

4. LOCAL CONSERVATION LAWS

It frequently occurs that locally defined quantities themselves are conserved as well as their sum over sites. This is called a local conservation law.[21] Figure 1 illustrates such an example in rule 73R, where once the three-site sequence

$$\begin{pmatrix} \hat{\sigma}_i & \hat{\sigma}_{i+1} & \hat{\sigma}_{i+2} \\ \sigma_i & \sigma_{i+1} & \sigma_{i+2} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

is present for some i, it continues to exist at the same place. Conversely, if a series of three sites does not show the above sequence at some time, it will never appear there. Accordingly, the quantity $(1-\sigma_i)(1-\hat{\sigma}_i)$ $\sigma_{i+1}\hat{\sigma}_{i+1}(1-\sigma_{i+2})(1-\hat{\sigma}_{i+2})$ is conserved for each i.

A local conservation law often causes walls which partition the system. In Fig. 1, the left and the right of the above sequence cannot communicate

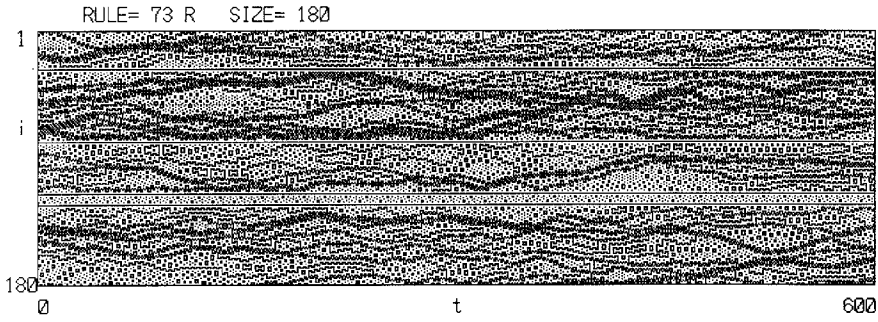

Fig. 1. An orbit $\{\sigma_i^t\}$ generated by rule 73R. Dots signify $\sigma_i^t = 1$ and blanks signify $\sigma_i^t = 0$. Four walls are seen.

any information through the sequence. If a temporally fixed or periodic pattern appears like this at a fixed position irrespective of its surroundings, it is called a wall. Some simple examples of the walls are illustrated in Fig. 2, and Table III shows the rules exhibiting them. Since every kind of sequence appears with some probability in a random initial configuration, a sufficiently large or an infinite system of such a rule is almost surely divided into a number of mutually noninteracting parts by walls. Such a system cannot show the mixing property. Thus, the walls prevent the statistical mechanics from being realized in principle.

Besides the rules shown in Table III, rules 27R and 59R have somewhat complicated walls. These rules have a common local conservation law which classifies all the two-site sequences into the two subsets

$$\Gamma_a = \left\{ \begin{pmatrix} \hat{\sigma}_i & \hat{\sigma}_{i+1} \\ \sigma_i & \sigma_{i+1} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \right\} \tag{4.1}$$

$$\Gamma_b = \left\{ \begin{pmatrix} \hat{\sigma}_i & \hat{\sigma}_{i+1} \\ \sigma_i & \sigma_{i+1} \end{pmatrix} \notin \Gamma_a \right\} \tag{4.2}$$

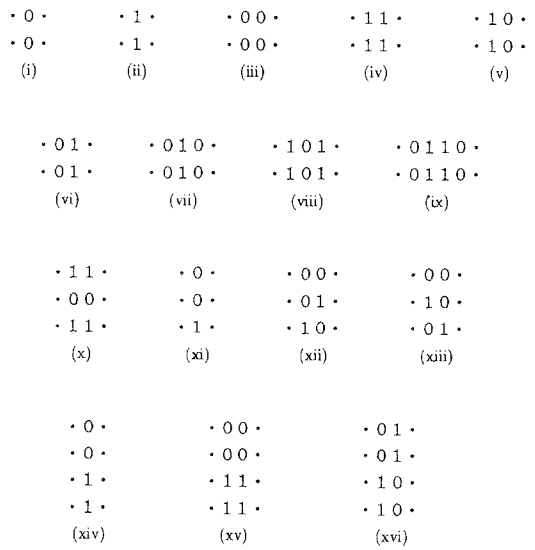

Fig. 2. Examples of wall configurations. Site number i increases from left to right, and time t downward. Dots mean arbitrary configurations.

Table III. Examples of the Walls[a]

Wall	Period	Rules
(i)	1	0R, 4R, 12R
(ii)	1	0R, 1R, 2R, 3R, 18R, 19R, 33R, 35R, 50R, 51R
(iii)	1	0R, 4R, 12R, 36R
(iv)	1	0R, 1R, 2R, 3R, 4R, 5R, 6R, 7R, 18R, 19R, 22R, 23R, 33R, 35R, 36R, 37R, 38R, 39R, 50R, 51R, 54R, 55R
(v)	1	0R, 1R, 2R, 3R, 9R, 10R, 11R, 129R, 131R, 139R
(vi)	1	0R, 1R, 129R
(vii)	1	0R, 1R, 9R, 73R, 129R
(viii)	1	0R, 1R, 2R, 3R, 18R, 19R, 129R, 131R, 147R
(ix)	1	0R, 1R, 4R, 5R, 129R, 133R
(x)	2	4R, 36R
(xi)	3	51R
(xii), (xiii)	3	51R, 179R
(xiv)	4	255R
(xv)	4	219R, 223R, 255R
(xvi)	4	126R, 127R, 255R

[a] For each of the wall configurations in Fig. 2 its period and rules exhibiting it are shown.

and only sequences belonging to one of these are seen at a fixed position. Consider a series of n sites where each couple of adjacent sites shows a sequence in Γ_a. Then, only the following six sequences are allowed to appear on such an n-site series:

$$\begin{pmatrix} \hat{\sigma}_i & \cdots & \hat{\sigma}_{i+n-1} \\ \sigma_i & \cdots & \sigma_{i+n-1} \end{pmatrix} = \begin{pmatrix} 0 & \cdots & 0 \\ 0 & \cdots & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & \cdots & 0 \\ 1 & \cdots & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & \cdots & 1 \\ 0 & \cdots & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 0 & \cdots & 0 \end{pmatrix} \tag{4.3}$$

All these sequences are homogeneous except for the leftmost site. Because $f(0, 0, 0) = 1$ and $f(1, 1, 1) = 0$ in rules 27R and 59R, orbits $\{\sigma_i^t\}$ inevitably behave like the following on such an n-site series:

$$\begin{array}{cccccc} * & 0 & 0 & \cdots & 0 \\ * & 0 & 0 & \cdots & 0 \\ * & 1 & 1 & \cdots & 1 \\ * & 0 & 0 & \cdots & 0 \\ * & 0 & 0 & \cdots & 0 \\ * & 1 & 1 & \cdots & 1 \end{array}$$

where time goes downward, i increases from left to right, and asterisks mean arbitrary symbols. Thus, except for the leftmost site, such an n-site series shows period three in time irrespective of the surroundings. This is the wall in rules 27R and 59R.

There are two rules which have a local conservation law but no walls, namely 24R and 46R. In these rules the propagation of energy is still inhibited. Rule 46R has the energy $(b_1, b_2, b_9, b_{11}, b_{12}) = (1, 1, -4, -4, 4)$, that is, the bond energy is written as

$$F^t_{i,i+1} = \sigma^t_i + \sigma^t_{i+1} + \hat{\sigma}^t_i + \hat{\sigma}^t_{i+1} - 4(\sigma^t_i + \hat{\sigma}^t_i)\,\sigma^t_{i+1}\hat{\sigma}^t_{i+1} + 4\sigma^t_i\hat{\sigma}^t_i\sigma^t_{i+1}\hat{\sigma}^t_{i+1} \tag{4.4}$$

The following gives the identical additive quantity Φ^t,

$$F^t_{i,i+1} = 1 - (1 - 2\sigma^t_i - 2\hat{\sigma}^t_i + 2\sigma^t_i\hat{\sigma}^t_i)(1 - \sigma^t_{i+1}\hat{\sigma}^t_{i+1}) \tag{4.5}$$

by the help of the arbitrariness of the additional terms (3.9). The flow corresponding to the bond energy (4.5) is given by

$$J^t_i = 2(1 - \hat{\sigma}^t_i)(1 - \sigma^t_i)(1 - \sigma^t_{i+1})\,f^t_i \tag{4.6}$$

However, since $f(0, 0, 0) = f(1, 0, 0) = 0$ for rule 46R, the above J^t_i indeed identically vanishes. Thus, the bond energy (4.5) itself is conserved for each bond $(i, i+1)$ and the initial arrangement of the energy does not change. Accordingly, no energy propagation can occur.

Things are more subtle in rule 24R. In this case, the energy of bond $(i, i+1)$ at time t is given by

$$F^t_{i,i+1} = (\sigma^t_i - \hat{\sigma}^t_{i+1})^2 + (\hat{\sigma}^t_i - \sigma^t_{i+1})^2 \tag{4.7}$$

and the flow at site i at time t is given by

$$J^t_i = (1 - 2\hat{\sigma}^t_i)(1 - 2\sigma^t_{i+1})\,f(\sigma^t_{i-1}, \sigma^t_i, \sigma^t_{i+1}) \tag{4.8}$$

The local conservation law for rule 24R classifies all two-site sequences into the two subsets

$$\Gamma_+ = \left\{ \begin{pmatrix} \hat{\sigma}_i & \hat{\sigma}_{i+1} \\ \sigma_i & \sigma_{i+1} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \right\} \tag{4.9}$$

$$\Gamma_- = \left\{ \begin{pmatrix} \hat{\sigma}_i & \hat{\sigma}_{i+1} \\ \sigma_i & \sigma_{i+1} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \right\} \tag{4.10}$$

and, similar to the case of rules 27R and 59R, a series of two sites can only show sequences in either of the above two subsets. Consider a series of three sites $(i-1, i, i+1)$, where the two-site series $(i-1, i)$ belongs to Γ_+ and $(i, i+1)$ to Γ_-. Twenty sequences are able to appear in such a three-site series. Out of these sequences, only the following can transfer the energy, i.e., have nonzero flow $J_i^t \neq 0$:

$$s_1 = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}, \quad s_2 = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$
$$s_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}, \quad s_4 = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \tag{4.11}$$

where $J_i^t = 1$ for s_1 and s_2, and -1 for s_3 and s_4. The point is that if the three-site series shows s_3 or s_4 at some time, it inevitably evolves into s_1 or s_2, respectively, at the next time step. Conversely, the only possible predecessors for s_1 and s_2 are s_3 and s_4, respectively. This imposes the following constraint for the transfer of the energy: If an energy passes through site i at some time, it must move back in the opposite direction at the next time step. Hence, the energy cannot propagate in substance through such a site. Things are similar if $(i-1, i)$ belongs to Γ_- and $(i, i+1)$ to Γ_+. On the other hand, if $(i-1, i)$ and $(i, i+1)$ belong to the same set, the energy can transfer through site i. Thus, in rule 24R, although bond energies do not directly give local conserved quantities, the energy propagation is still prevented.

The existence of a local conservation law is equivalent to a lack of n-site sequences appearing at a fixed position in a run starting from an arbitrary configuration. In a rule without a local conservation law, all the 4^n sequences can appear; in other words, the value of the spatial set entropy[22] is unity for any n. In contrast with this, in a rule with a local conservation law, the set of n-site sequences with some n is classified into a number of subsets and at a fixed position there only appear sequences belonging to one among them.

This situation can be represented in terms of a transition matrix as follows. An n-site sequence $x_n = (\sigma_1, ..., \sigma_n, \hat{\sigma}_1, ..., \hat{\sigma}_n)$ evolves in unit time step into one of the following sequences:

$$\{(f(\alpha, \sigma_1, \sigma_2) \text{ XOR } \hat{\sigma}_1, ..., f(\sigma_{n-1}, \sigma_n, \beta) \text{ XOR } \hat{\sigma}_n, \sigma_1, ..., \sigma_n): \quad \alpha, \beta \in \{0, 1\}\} \tag{4.12}$$

the number of which is at most four. If the evolution from x_n to x_n' is allowed in the above sense, one sets the element $T_{x_n, x_n'}$ of the $4^n \times 4^n$ matrix T unity, and zero otherwise. Then the existence of a local conservation law is equivalent to the reducibility of the transition matrix T.

Examination of the above property has been carried out for the 88 classes of the rules. The result in the case of $n=4$ indicates the existence of a local conservation law for 44 classes of rules, which have already appeared in Table III or in the text, and the lack of it for the remaining 44 classes. The result does not change for $n=5$ and 6. When $n<4$, however, one fails to notice the existence of a local conservation law in rule 133R, where the sequence

$$\begin{pmatrix} \hat{\sigma}_i & \hat{\sigma}_{i+1} & \hat{\sigma}_{i+2} & \hat{\sigma}_{i+3} \\ \sigma_i & \sigma_{i+1} & \sigma_{i+2} & \sigma_{i+3} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

acts as a wall. These observations strongly suggest that the latter 44 classes are not accompanied by a local conservation law for any n. I conjecture that in general a family of reversible cellular automata of the Fredkin construction type has a threshold size of block determined by the interaction range such that if a rule in the family does not show a local conservation law for that block, it has none for any size of blocks. In the case of ERCAs the threshold is given by $n=4$. This is the same as the statement that a local conservation law is literally a local property of a rule. If this conjecture is true, one can determine whether a local conservation law exists or not by a finite procedure. Though this conjecture seems plausible, I have no mathematical proof for it.

Both the existence of an additive conserved quantity (energy) and the lack of local conservation laws are necessary for statistical mechanics to hold. Rules potentially satisfying both these conditions are listed in Table IV along with their energy functions F. These rules do not have any local conservation laws at least up to $n=6$ and never if the above conjecture is true. It is numerically observed that the energies can propagate indefinitely in these rules. Note that all these functions only take three possible values [0, 1, 2 for energies (a) and (b) and -1, 0, 1 for (c) and

Table IV. Rules with Propagative Energy[a]

Rules	Additive invariants: $F(\alpha, \beta, \hat{\alpha}, \hat{\beta})$
26R	(a): $(\alpha-\hat{\beta})^2+(\hat{\alpha}-\beta)^2$
90R	(a), (d): $\alpha\hat{\beta}-\hat{\alpha}\beta$ [or $(\hat{\alpha}-\beta)^2-(\alpha-\hat{\beta})^2$]
91R, 123R	(b): $1+\alpha\hat{\alpha}+\beta\hat{\beta}-[1-2(1-\alpha)(1-\hat{\beta})][1-2(1-\hat{\alpha})(1-\beta)]$ and (d)
77R	(c): $\alpha\hat{\beta}(1-2\hat{\alpha}-2\beta)-\hat{\alpha}\beta(1-2\alpha-2\hat{\beta})$
94R, 95R	(d)

[a] Rules having an additive invariant of the form (3.1) but no local conservation laws. Energy (d) is shown with two kinds of representations.

(d)]. Furthermore, (a) and (b) are symmetric with respect to the reflection and the exchange of variables $(\alpha, \beta) \leftrightarrow (\hat{\alpha}, \hat{\beta})$, but (c) and (d) are antisymmetric under either of these transformations. These rules are extensively investigated in the subsequent papers concerning thermodynamic properties.

5. PHASE SPACE STRUCTURE

The phase space for a finite ERCA is divided into a number of cycles under the periodic boundary condition, because the number of distinct states is finite and the time evolution is reversible. Hence, the distribution of cycle lengths provides fundamental information about the phase space structure and ergodic nature of ERCAs. In this section, I discuss system-size dependence of the distribution, particularly of the number of cycles and the mean cycle length (the expected value for the cycle length). Since additive rules and their complements have a distinct property, they are treated separately from others.

Additive rules satisfy the additive superposition law, that is, if $\{\boldsymbol{\alpha}^t\}$ and $\{\boldsymbol{\beta}^t\}$ are two orbits in such a rule, $\{\boldsymbol{\alpha}^t \text{ XOR } \boldsymbol{\beta}^t\}$ also becomes an orbit in the rule. The complements of additive rules also show a type of superposition law, as discussed in Appendix A. By virtue of these superposition laws, there is an algebraic method with which time evolution of a given initial configuration is written in a compact form and in turn the distribution of cycle lengths can be obtained.[23] However, it may be actually too hard to be carried out in the present case. Then I made simpler use of the additivity. In such a rule, the orbit starting from a basis configuration for the superposition law, where only one element of $\{\sigma_i\}$ or $\{\hat{\sigma}_i\}$ is unity and others are zeros, gives the common fundamental cycle length. And a cycle length becomes short only when some degeneracy occurs. Thus, the maximal cycle length for each value of size N is easily obtainable with a numerical method. I carried this out for systems with size $N < 29$. The result shows the following three types of behavior. First, rules 0R, 51R, and 255R have the cycle lengths independent of N, because the time evolution of variables on each site is independent of other sites in these rules. Second, rules 15R, 60R, 105R, and 153R show an apparently irregular N dependence, reflecting some number-theoretic property of N. Figure 3 illustrates the case of rule 15R. Lastly, the maximal cycle lengths in rules 90R and 165R show globally linear increase in N, though having some local structure. Since the volume of the phase space is 4^N, in the first and third cases the number of cycles shows exponential increase of order $O(4^N)$ and $O(4^N/N)$, respectively.

Rules other than the above have no such useful properties. For

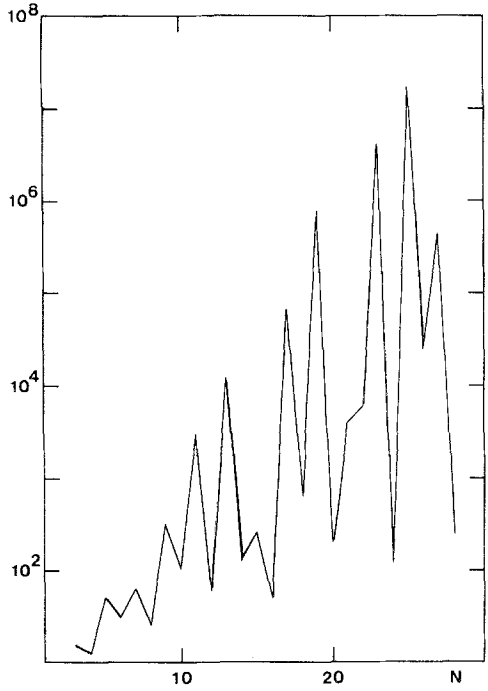

Fig. 3. Maximal cycle length as a function of system size for rule 15R, exhibiting number-theoretic irregular behavior.

systems with relatively small size N, however, it is still possible to investigate all the states in the phase space to enumerate the cycles exactly. In this way, the distributions of cycle lengths were obtained for the 88 classes with $N \leqslant 13$. As a result, it has been found that for almost all rules except those showing the number-theoretic irregularity mentioned above, the numbers of cycles commonly increase exponentially like $2^N \sim 4^N$. In particular, it is $O(2^N)$ for rules with no (additive or local) conservation laws. See Fig. 4. On the other hand, the mean or maximal cycle length shows a rich variety of N dependence from constant to exponential. The exponential increase of the number of cycles is large compared with the average number of cycles for random substitutions,[24] which predicts the logarithm of the phase space volume, accordingly linear increase in N. That the exponential increase is commonly seen is probably due to the time-reversal invariance of ERCAs. This is suggested by the fact that Wolfram's elementary rule 45, which is reversible but not time-reversal invariant in case of odd N, shows the mean cycle length of $O(2^N)$, proportional to the phase space volume in this case. The number of cycles in rule 45 seems not to increase as fast as in ERCAs.

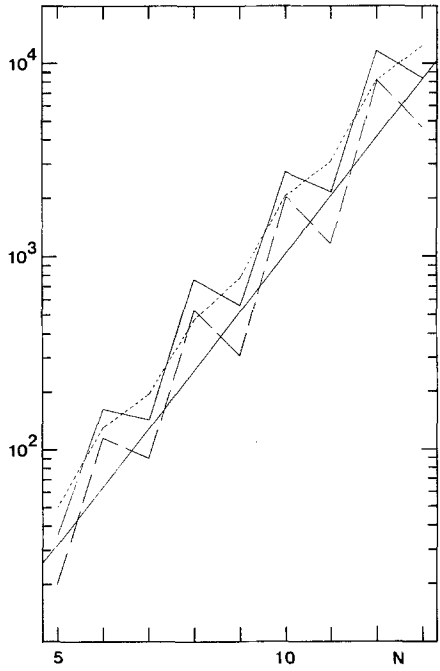

Fig. 4. Number of cycles for three rules having no additive or local conservation laws, 30R (dotted line), 75R (solid line), and 155R (broken line). The straight line represents 2^N.

The exponential increase of the number of cycles has a significant meaning for the ergodic nature of ERCAs, because this fact indicates that a finite ERCA is not ergodic in the strict sense. The number of possible values of an energy (additive conserved quantity) is proportional to N. Hence, if a rule has more than one energy, the number of possible values for the energies is at most a constant times a power of N. The exponential increase, therefore, means that a huge number of distinct orbits coexist on an energy surface. This means the lack of ergodicity in the strict sense. Though a set of local conserved quantities may be used to label the orbits, thermodynamic behavior cannot be expected for such rules, as has been discussed in Section 4.

The above nonergodicity does not necessarily indicate the absence of thermodynamic behavior of the models. It is mathematically proved that the noninteracting ideal gas is nonergodic in finite systems but Bernoulli (accordingly ergodic) in an infinite system. Such a recovery of ergodicity in an infinite system may be expected also in the case of ERCAs. Indeed, rule 90R can be identified with a kind of noninteracting ideal gas system because a unit of the energy (a) in Table IV moves with velocity ± 1

irrespective of other units of the energy.[6] If the recovery of ergodicity really occurs in ERCAs, thermodynamic behavior will be realized in some respects in a large system.

6. SUMMARY AND DISCUSSION

In this paper I have presented a family of one-dimensional reversible cellular automata named ERCAs and investigated basic properties in preparation for the study of thermodynamic behavior of large systems. After the classification according to symmetry properties, energy was introduced as an additive invariant of the form (3.1). The existence of a local conservation law, which prevents the realization of statistical mechanics, was examined for each class of the rules. In this way rules which have at least one additive conserved quantity but no local conservation laws have been selected as hopeful candidates for thermodynamic behavior. The distribution of cycle lengths was investigated by exact enumeration for relatively small systems, which has revealed the coexistence of a huge number of orbits on an energy surface.

Symmetry and conservation laws are the most fundamental properties for all physical systems. Thus, the results obtained here will provide basic data for any study using ERCAs. For example, a nonadditive rule possessing no additive or local conservation laws generates a pattern $\{\sigma_i^t\}$ characteristic of the rule, which does not depend on the initial conditions so much. On the other hand, patterns generated by rules possessing conservation laws strongly depend on the initial conditions.

Though I have obtained the complete list for the additive conserved quantities of the form (3.1), there are possibilities for other types of additive invariants to exist. Table II is obtained through a straightforward calculation, but the search in this manner becomes tedious when more quantities are involved. Thus, to proceed further, one must solve the question of what algebraic property is the origin of additive conserved quantities.

The distribution of cycles predicts the nonergodicity of ERCAs. The coexistence of cycles on an energy surface means that there exists some conserved quantity other than Φ. For example, if different values are assigned for different orbits, the values are conserved. However, such a quantity is not necessarily an additive one and may not even be written in a compact form. Thus, it is possible that every such orbit shows a similar behavior with regard to thermodynamic quantities. Furthermore, since the present result is obtained for relatively small systems, there remains the possibility that the size dependence of the cycle distribution might change in large systems.

The rules in Table IV have additive conserved quantities with which statistical mechanics can be constructed. Moreover, no local conservation laws are found for these rules and there seems nothing to inhibit the energy propagation. Thus, thermodynamic behavior may be expected. In the subsequent papers, these rules will be investigated with respect to equilibrium and nonequilibrium thermodynamic behavior.

APPENDIX A. THE SYMMETRY OF COMPLEMENT

Rule $\bar{f}$R specified by the Boolean function $\bar{f}$ is said to be the complement of rule fR if the functions are connected by the relation $\bar{f} = 1 - f$. Hereafter the bar denotes the binary complement operation for the Booleans. In contrast with the reflection and the Boolean conjugation symmetries, the complement does not generally yield isomorphisms between rules. In cases that a certain condition is satisfied, however, it brings such interesting consequences as some correspondences between orbits in *even* or *odd* rules, a periodically varying additive quantity for a group of rules, and some kinds of superposition laws for orbits in the complements of additive rules. In this Appendix, I explain these in order.

First, I discuss the orbit correspondence in even and odd rules. Let rules hR and $\bar{h}$R be the rule conjugate to fR and its complement, respectively. Namely, $h(\mu, \nu, \kappa) = f(\bar{\mu}, \bar{\nu}, \bar{\kappa})$ and $\bar{h} = 1 - h$. Then, for an orbit $\{\boldsymbol{\sigma}^t\}$ in rule fR, the following equations hold:

$$\begin{aligned} \boldsymbol{\sigma}^{t+1} &= \mathbf{f}(\boldsymbol{\sigma}^t)\ \mathrm{XOR}\ \boldsymbol{\sigma}^{t-1} \\ &= \bar{\mathbf{f}}(\boldsymbol{\sigma}^t)\ \mathrm{XOR}\ \overline{\boldsymbol{\sigma}^{t-1}} \\ &= \mathbf{h}(\overline{\boldsymbol{\sigma}^t})\ \mathrm{XOR}\ \boldsymbol{\sigma}^{t-1} \\ &= \bar{\mathbf{h}}(\overline{\boldsymbol{\sigma}^t})\ \mathrm{XOR}\ \overline{\boldsymbol{\sigma}^{t-1}} \end{aligned} \tag{A.1}$$

Hence, if a set $\{\boldsymbol{\lambda}^t\}$ is defined by

$$\begin{aligned} \boldsymbol{\lambda}^t &= \boldsymbol{\sigma}^t \qquad \text{for} \quad t = 0 \text{ or } 1 \pmod 4 \\ \boldsymbol{\lambda}^t &= \overline{\boldsymbol{\sigma}^t} \qquad \text{for} \quad t = 2 \text{ or } 3 \pmod 4 \end{aligned} \tag{A.2}$$

these $\boldsymbol{\lambda}^t$ satisfy

$$\begin{aligned} \boldsymbol{\lambda}^{t+1} &= \bar{\mathbf{f}}(\boldsymbol{\lambda}^t)\ \mathrm{XOR}\ \boldsymbol{\lambda}^{t-1} \qquad \text{for} \quad t = 0 \text{ or } 1 \pmod 4 \\ \boldsymbol{\lambda}^{t+1} &= \bar{\mathbf{h}}(\boldsymbol{\lambda}^t)\ \mathrm{XOR}\ \boldsymbol{\lambda}^{t-1} \qquad \text{for} \quad t = 2 \text{ or } 3 \pmod 4 \end{aligned} \tag{A.3}$$

This is a general relation valid for any reversible cellular automata of Fredkin construction type.

In the case that the rule is invariant under the Boolean conjugation, that is, $h=f$, Eq. (A.3) implies that $\{\lambda^t\}$ is an orbit in rule $\bar{f}$R. Rules possessing this property are said to be *even* or self-conjugate.[11] As found from Table I, the self-conjugate classes and their complements are the following six pairs:

$$\begin{aligned} &[0\text{R}] \leftrightarrow [255\text{R}], \quad [24\text{R}] \leftrightarrow [189\text{R}], \quad [36\text{R}] \leftrightarrow [219\text{R}], \\ &[60\text{R}] \leftrightarrow [153\text{R}], \quad [90\text{R}] \leftrightarrow [165\text{R}], \quad [126\text{R}] \leftrightarrow [129\text{R}]. \end{aligned} \tag{A.4}$$

A pair of these corresponding rules has similar phase space structure. This is because periods of corresponding orbits are not necessarily the same, but are connected by the following relations: If period T for an orbit is odd, that for the corresponding orbit is $2T$ or $4T$; if T is a multiple of four, the corresponding period is T or $T/2$ or $T/4$; and if $T=2 \pmod 4$, the corresponding period is $2T$ or $T/2$. These relations are a direct result from Eq. (A.3).

Self-conjugate rules have another correspondence. Consider the case that the number of sites N is even and the system has the periodic boundary condition. The (i, t) plane is divided into two parts like the checkerboard according as $i+t$ is even or odd. If one applies the Boolean conjugation on one part of the checkerboard, i.e.,

$$\begin{aligned} \rho_i^t &= \sigma_i^t \quad \text{if} \quad i+t=\text{even} \\ \rho_i^t &= \overline{\sigma_i^t} \quad \text{if} \quad i+t=\text{odd} \end{aligned} \tag{A.5}$$

then $\{\boldsymbol{\rho}^t\}$ becomes an orbit in rule gR where the function g is defined by

$$g(\mu, \nu, \kappa) = f(\bar{\mu}, \nu, \bar{\kappa}) = f(\mu, \bar{\nu}, \kappa) \tag{A.6}$$

The second equality means the self-conjugate condition. This transformation yields the correspondences between the classes

$$[36\text{R}] \leftrightarrow [129\text{R}], \quad [60\text{R}] \leftrightarrow [153\text{R}], \quad [126\text{R}] \leftrightarrow [219\text{R}] \tag{A.7}$$

and other self-conjugate classes have rule correspondences within each class. Each pair of rules in (A.7) has an identical phase space structure when N is even.

Equation (A.1) yields another useful transformation. If a set $\{\boldsymbol{\chi}^t\}$ is defined from $\{\boldsymbol{\sigma}^t\}$ by

$$\begin{aligned} \boldsymbol{\chi}^t &= \boldsymbol{\sigma}^t \quad \text{for} \quad t=0 \text{ or } 1 \pmod 3 \\ \boldsymbol{\chi}^t &= \overline{\boldsymbol{\sigma}^t} \quad \text{for} \quad t=2 \pmod 3 \end{aligned} \tag{A.8}$$

it satisfies the equations

$$\begin{aligned} \chi^{t+1} &= \bar{f}(\chi^t)\ \mathrm{XOR}\ \chi^{t-1} \qquad \text{for} \quad t = 0 \text{ or } 1 \pmod 3 \\ \chi^{t+1} &= \bar{h}(\chi^t)\ \mathrm{XOR}\ \chi^{t-1} \qquad \text{for} \quad t = 2 \pmod 3 \end{aligned} \tag{A.9}$$

This is also a general relation.

If the complement coincides with the conjugate, namely $h = \bar{f}$, $\{\chi^t\}$ is an orbit in rule $\bar{f}$R. Rules with this property are called *odd*.[11] There are six classes of odd rules. In addition, the conjugates coincide with the reflections of complements in two classes, which should be included in the odd case. Thus, the odd classes are

$$[15\mathrm{R}],\quad [23\mathrm{R}],\quad [29\mathrm{R}],\quad [43\mathrm{R}],\quad [51\mathrm{R}],\quad [57\mathrm{R}],\quad [77\mathrm{R}],\quad [105\mathrm{R}] \tag{A.10}$$

where [29R] and [57R] are the latter cases. Contrary to the self-conjugate cases, the orbit correspondence between odd rules is limited within the same class.

It should be noticed that the complement symmetry yields the correspondences between orbits with the same initial configuration in both the even and the odd cases, while the orbit correspondences based on the reflection or the Boolean conjugation symmetry are between orbits with transformed initial conditions.

Next, I discuss a relation between the complement symmetry and an additive quantity. For some rules a periodically varying additive quantity can be found by utilizing Eq. (A.3). Consider the case that rules $\bar{f}$R and $\bar{h}$R have a common additive conserved quantity $\Phi(x)$. Then, from Eq. (A.3), $\Phi(\boldsymbol{\lambda}^t, \hat{\boldsymbol{\lambda}}^t) = \text{const}$, which means that $\Phi(\boldsymbol{\sigma}^t, \hat{\boldsymbol{\sigma}}^t)$ is periodic with period at most four. Furthermore, if Φ is self-conjugate, i.e., $\Phi(\bar{x}) = \Phi(x)$, the period becomes at most two. This is the case for rules 165R, 167R, 175R, 183R, 189R, and 191R with $\Phi(x) = \sum_i \{(\sigma_i - \hat{\sigma}_{i+1})^2 + (\hat{\sigma}_i - \sigma_{i+1})^2\}$. As is stated in Section 3, this Φ is conserved for the rules in classes [90R], [26R], [24R], [18R], [10R], [4R], [2R], and [0R]. For example, the complement of rule 167R is rule 88R, which belongs to class [26R], and the conjugate of the complement is rule 26R itself. Similar things are realized in other cases.

Finally, superposition laws utilizing the complement property are considered. When the function f is written with XOR only, rule fR is called additive. By this definition, an additive rule is necessarily either even or odd. Thus, Eq. (A.2) or (A.8) transforms an orbit into one in the complement rule and vice versa. Utilizing this fact, one can derive a kind of superposition law for the complements of additive rules as follows.

Let $\{\boldsymbol{\alpha}^t\}$ and $\{\boldsymbol{\beta}^t\}$ be orbits in the complement of an additive rule, and $\{\boldsymbol{\sigma}^t\}$ and $\{\boldsymbol{\mu}^t\}$ be their transforms given by Eq. (A.2) or (A.8) according to whether the rule is even or odd, respectively. By the definition of the additive rule, $\{\boldsymbol{\sigma}^t \text{ XOR } \boldsymbol{\mu}^t\}$ is also an orbit in the rule. Then the inverse transformation of $\{\boldsymbol{\sigma}^t \text{ XOR } \boldsymbol{\mu}^t\}$ yields the following superposition laws for the complements: From two orbits $\{\boldsymbol{\alpha}^t\}$ and $\{\boldsymbol{\beta}^t\}$, an orbit $\{\boldsymbol{\gamma}^t\}$ is generated by

$$\begin{aligned} \boldsymbol{\gamma}^t &= \boldsymbol{\alpha}^t \text{ XOR } \boldsymbol{\beta}^t \qquad \text{for} \quad t = 0 \text{ or } 1 \pmod 4 \\ \boldsymbol{\gamma}^t &= \overline{\boldsymbol{\alpha}^t \text{ XOR } \boldsymbol{\beta}^t} \qquad \text{for} \quad t = 2 \text{ or } 3 \pmod 4 \end{aligned} \tag{A.11}$$

for an even case, and by

$$\boldsymbol{\gamma}^t = \overline{\boldsymbol{\alpha}^t \text{ XOR } \boldsymbol{\beta}^t} \qquad \text{for all } t \tag{A.12}$$

for an odd case. In the even classes (A.4), [0R], [60R], and [90R] are additive and [255R], [153R], and [165R] are their complements, respectively. In the odd case, classes [15R], [51R], and [105R] contain an additive rule and its complement in each.

APPENDIX B. DERIVATION OF (3.6)

In this Appendix, I show that Eqs. (3.6a)–(3.6e) are the necessary and sufficient conditions for Eq. (3.1) to be invariant, i.e.,

$$\delta\Phi^t \equiv \Phi^{t+1} - \Phi^t = 0 \tag{B.1}$$

where $\Phi^t = \sum_i F(\sigma_i^t, \sigma_{i+1}^t, \hat{\sigma}_i^t, \hat{\sigma}_{i+1}^t)$. Representing the variables at time $t+1$ by those at time t and substituting the general form (3.5) for F into Eq. (B.1), one has

$$\begin{aligned} \delta\Phi = \sum_i \{ & 2(b_1 - b_2)(\hat{\sigma}_i - \sigma_i) + (b_3 - b_4)(\hat{\sigma}_i\hat{\sigma}_{i+1} - \sigma_i\sigma_{i+1}) \\ & + (b_6 - b_7)(\hat{\sigma}_i\sigma_{i+1} - \sigma_i\hat{\sigma}_{i+1}) \\ & + (b_8 - b_{10})\,\sigma_i\hat{\sigma}_i(\hat{\sigma}_{i+1} - \sigma_{i+1}) + (b_9 - b_{11})\,\sigma_{i+1}\hat{\sigma}_{i+1}(\hat{\sigma}_i - \sigma_i) \\ & + (1 - 2\hat{\sigma}_i)\, f_i[2b_1 + b_3(\hat{\sigma}_{i-1} + \hat{\sigma}_{i+1}) + 2b_5\sigma_i + b_6\sigma_{i+1} + b_7\sigma_{i-1} \\ & + b_8(\sigma_{i-1}\hat{\sigma}_{i-1} + \sigma_i\hat{\sigma}_{i+1}) + b_9(\sigma_i\hat{\sigma}_{i-1} + \sigma_{i+1}\hat{\sigma}_{i+1}) + b_{10}\sigma_i\sigma_{i+1} \\ & + b_{11}\sigma_{i-1}\sigma_i + b_{12}(\sigma_{i-1}\sigma_i\hat{\sigma}_{i-1} + \sigma_i\sigma_{i+1}\hat{\sigma}_{i+1})] \\ & + (1 - 2\hat{\sigma}_i)(1 - 2\hat{\sigma}_{i+1})\, f_i f_{i+1}[b_3 + b_8\sigma_i + b_9\sigma_{i+1} + b_{12}\sigma_i\sigma_{i+1}]\} \end{aligned} \tag{B.2}$$

where the index t is omitted to avoid confusion. Equation (B.1) requires Eq. (B.2) to vanish identically. In particular, the following has to be satisfied:

$$\begin{aligned}
&\delta\Phi(\hat{\sigma}_i=0)-\delta\Phi(\hat{\sigma}_i=1)\\
&\quad=\{-2(b_1-b_2)-(b_6-b_7)(\sigma_{i+1}-\sigma_{i-1})\\
&\qquad+(b_8-b_{10})\,\sigma_i\sigma_{i+1}+(b_9-b_{11})\,\sigma_{i-1}\sigma_i\\
&\qquad+2f_i[2b_1+2b_5\sigma_i+b_6\sigma_{i+1}+b_7\sigma_{i-1}+b_{10}\sigma_i\sigma_{i+1}+b_{11}\sigma_{i-1}\sigma_i]\\
&\qquad-(1-2f_i)\,f_{i+1}[b_3+b_8\sigma_i+b_9\sigma_{i+1}+b_{12}\sigma_i\sigma_{i+1}]\\
&\qquad-(1-2f_i)\,f_{i-1}[b_3+b_8\sigma_{i-1}+b_9\sigma_i+b_{12}\sigma_{i-1}\sigma_i]\}\\
&\qquad+\hat{\sigma}_{i-1}\{-(b_3-b_4)-(b_8-b_{10})\,\sigma_{i-1}-(b_9-b_{11})\,\sigma_i\\
&\qquad+2(f_{i-1}-f_i)^2\,(b_3+b_8\sigma_{i-1}+b_9\sigma_i+b_{12}\sigma_{i-1}\sigma_i)\}\\
&\qquad+\hat{\sigma}_{i+1}\{-(b_3-b_4)-(b_8-b_{10})\,\sigma_i-(b_9-b_{11})\,\sigma_{i+1}\\
&\qquad+2(f_i-f_{i+1})^2\,(b_3+b_8\sigma_i+b_9\sigma_{i+1}+b_{12}\sigma_{i+1})\}\\
&\quad=0
\end{aligned}\tag{B.3}$$

Since this must be identically zero, three curly brackets turn out to vanish separately. From the second or the third, one has a set of equations for $\{b_i\}$ as

$$\begin{aligned}
&2(b_3+b_8\sigma_i+b_9\sigma_{i+1}+b_{12}\sigma_i\sigma_{i+1})(f_i-f_{i+1})^2\\
&\qquad=b_3-b_4+(b_8-b_{10})\,\sigma_i+(b_9-b_{11})\,\sigma_{i+1}
\end{aligned}\tag{B.4}$$

If one puts $\sigma_{i-1}=\sigma_i=\sigma_{i+1}=\sigma_{i+2}$, the left-hand side of the above equation vanishes since $f_i=f_{i+1}$ in such cases. Thus, Eqs. (3.6b) and (3.6c) are derived. Substitution of Eqs. (3.6b) and (3.6c) into Eq. (B.4) yields Eq. (3.6d). The vanishing condition for the first curly bracket in Eq. (B.3) gives Eq. (3.6e) with the help of Eqs. (3.6b)–(3.6d), though at this stage the term $2(b_1-b_2)$ remains to be added to the right-hand side of Eq. (3.6e). The equations thus obtained are the condition for Eq. (B.3) to hold and only a necessary condition for $\delta\Phi$ to vanish. Using Eq. (B.3) repeatedly, one has

$$\delta\Phi(\boldsymbol{\sigma},\hat{\boldsymbol{\sigma}})=\delta\Phi(\boldsymbol{\sigma},\hat{\boldsymbol{\sigma}}=\mathbf{0}) \tag{B.5}$$

By the help of this and the equations obtained above, one can rewrite $\delta\Phi$ as

$$\delta\Phi=(b_1-b_2)\sum_i(1-2\sigma_i). \tag{B.6}$$

For this to be identically zero, the condition (3.6a) is necessary and sufficient. Thus, one arrives at Eqs. (3.6a)–(3.6e).

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