PHYSICAL REVIEW LETTERS

VOLUME 59 | 30 NOVEMBER 1987 | NUMBER 22

Reversible Cellular Automata and Statistical Mechanics

Shinji Takesue
Institute of Physics, College of Arts and Sciences, University of Tokyo, Tokyo 153, Japan
(Received 21 May 1987)

Reversible cellular automata are used to investigate the thermodynamic behavior of large systems. Additive conserved quantities are regarded as the energy of these models. By the consideration of a large system as the sum of a subsystem and a heat bath, it is numerically shown that a canonical distribution is realized under certain conditions concerning the conserved quantities.

PACS numbers: 05.20.−y, 02.50.+s, 05.45.+b

The foundation of statistical mechanics has not been established as yet. Ergodicity is not generic for classical mechanical systems with a finite number of degrees of freedom, as the Kolmogorov-Arnol'd-Moser theory has revealed.[1] In addition, if a finite system is not ergodic, the same kind of infinite system can be ergodic. The noninteracting ideal gas[2] and the complete harmonic crystal[3] give such examples. No general theorem is known for the ergodicity of infinite systems.

Reversible cellular automata provide us with clear examples to investigate the problem.[4] A cellular automaton is a dynamical system composed of discrete variables on a discrete space-time. The states of all the variables are synchronously updated at every time step according to a definite rule, which is locally defined and uniform in space. If a cellular automaton is reversible, that is, if each configuration has a unique predecessor, it automatically satisfies the Liouville theorem by virtue of the discreteness of the variables. Consequently, the statistical mechanics of the model can formally be constructed, provided that it has a conserved quantity which can be regarded as a kind of energy. The existence of such quantities has been shown by Pomeau[5] for a particular type of reversible cellular automata. Then a direct comparison is possible between the results of the statistical mechanics (ensemble average) and those of the dynamics (time average).

Moreover, such investigation justifies the recently advanced applications of cellular automata as computational tools. The features of cellular automata are strikingly suitable for execution by digital computers. In particular, fast simulations are possible without round-off errors. Taking advantage of this, a deterministic Ising dynamics has been devised for Monte Carlo calculations,[6] and lattice-gas automata for simulations of the Navier-Stokes equation.[7] 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 the microscopic level. Nevertheless, their macroscopic nature is expected to be physical, provided that they show standard thermodynamic behaviors, such as canonical distribution, local equilibrium, and the Green-Kubo formula. Although successful simulation results have been reported,[8] it has not been clarified for what conditions the thermodynamic behavior is realized. This is just the problem which I will consider.

In this Letter, I concentrate on the realization of equilibrium statistical mechanics (canonical distribution). I define a set of reversible cellular automata and classify them with respect to a kind of additive conserved quantity. It is shown that the canonical distribution is realized for a certain class of reversible cellular automata and their conserved quantities.

The models I deal with are the one-dimensional reversible cellular automata whose local rules are of the form[4]

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

$$\hat{\sigma}_i^{t+1} = \sigma_i^t, \quad (2)$$

where σ_i^t and $\hat{\sigma}_i^t$ are Boolean variables of site i at time t which may take values 0 or 1, f denotes a Boolean function of three variables, and XOR means the "exclusive OR" operation. I call these models elementary reversible cellular automata (ERCA). The phase space is defined for ERCA with N sites, where I usually impose the cyclic boundary condition to keep the reversibility, as the set of configurations $(\sigma_1, \hat{\sigma}_1, \ldots, \sigma_N, \hat{\sigma}_N)$. Thus the phase space has 4^N configurations in it. Notice that the time-reversed evolution is obtained with the same rule by an exchange between the σ's and $\hat{\sigma}$'s for a configuration. This means that ERCA are not only reversible but also time-reversal invariant as are classical mechanical systems.

There exist $2^{2^3} = 256$ distinct Boolean functions of three variables and accordingly as many ERCA. I denote each ERCA by the number $\sum_{\mu,\nu,\kappa} 2^{4\mu+2\nu+\kappa} \times f(\mu,\nu,\kappa)$, specifying f in Wolfram's convention,[9] and an R appended to it. Thus, for example, if $f(x,y,z) = x \,\mathrm{XOR}\, z$, the ERCA is called $90R$. Symmetries concerning reflection (left-right symmetry) and Boolean conjugation classify the set of ERCA into 88 equivalence classes, in each of which corresponding orbits of different ERCA are transformed into each other by the symmetry transformations. The properties considered in this Letter are qualitatively unaffected by the transformations. Hence, I consider only the minimal-numbered representatives of each class.

To construct the statistical mechanics of ERCA, energy has to be introduced. Since an ERCA does not have an *a priori* Hamiltonian, I define the energy as a conserved quantity which is additive and propagative.

The additivity means that the energy must be written as a sum of identical functions of local variables over all sites. I have examined, therefore, the following additive quantities as candidates for the energy of ERCA:

$$\Phi = \sum_i F(\sigma_i, \sigma_{i+1}, \hat{\sigma}_i, \hat{\sigma}_{i+1}), \quad (3)$$

where F is an appropriate function chosen according to the rule of ERCA. While the restriction that the function F depend only upon two neighboring sites is made for simplicity, it equips the quantity Φ with the picture that the bond $(i, i+1)$ has an energy

$$F_{i,i+1} = F(\sigma_i, \sigma_{i+1}, \hat{\sigma}_i, \hat{\sigma}_{i+1}).$$

The capability of propagation is connected with the nonexistence of local conservation laws. When a locally defined quantity does not depend on time, the system is said to satisfy the local conservation law. Depending on its value, such a quantity often acts as a "wall" beyond which no information can propagate.[10] Clearly the presence of such walls obstructs the realization of the statistical mechanics. The number of conserved quantities is too many in such cases.

I carried out the classification of ERCA in terms of the presence of additive conserved quantities and walls. The conservation of Φ was examined by straightforward calculation with use of a polynomial expansion of F. The presence of walls was checked both numerically and analytically. As the result, I have obtained the following three types: (i) no additive conserved quantities written as (3) exist (this type contains 41 classes); (ii) additive conserved quantities exist, but not local conservation laws which lead to walls (7 classes); (iii) both additive conserved quantities and walls exist (40 classes).

To see the realization of equilibrium statistical mechanics, I numerically examined the distribution function for the energy of a subsystem in the following manner. Consider a large system of size N with the periodic boundary condition. A particular series of n $(\ll N)$ bonds is distinguished as a subsystem from the remaining part, which is regarded as a heat bath. The energy of the subsystem is given by the sum of energies assigned to the n bonds. The density of states $D(E)$ is calculated as $D(E) = 4^{-n-1} \times$(the number of configurations with the subsystem's energy E) by examination of the 4^{n+1} possible configurations for the subsystem. Then, according to statistical mechanics, the distribution function for the energy of the subsystem $P(E)$ should be asymptotically proportional to $D(E)e^{-\beta E}$ in the limit as $N, n \to \infty$ $(N \gg n)$ with the energy density $\phi = \Phi/N$ fixed. Furthermore, the inverse temperature β is determined by the relation $\phi = -(\partial/\partial\beta)\ln Z$ through the partition function $Z = \sum e^{-\beta\Phi}$. In particular, the relation is obtained as $\beta = \ln[(2-\phi)/\phi]$ for the energy (3). Thereby I calculated $P(E)$ in a run with T iteration steps as $P(E) = T^{-1} \times$(the number of time steps with the subsystem's energy E), where the run started from a random configuration with given total energy Φ. Then, the linearity of $\ln[P(E)/D(E)]$ vs E was checked, and the slope $-\beta$ was compared with the analytical result of the statistical mechanics.

Only the type-2 ERCA have the possibility of thermodynamic behavior. As a matter of fact, I have found that the canonical distribution is realized for the energy type-2 ERCA. In the following, I illustrate this by adducing examples.

The quantity Φ, given by (3) with the function

$$F(x,y,\hat{x},\hat{y}) = (x-\hat{y})^2 + (\hat{x}-y)^2, \quad (4)$$

is conserved for the equivalence classes represented by rules $0R$, $2R$, $4R$, $10R$, $18R$, $24R$, $26R$, and $90R$. For the former six rules local conservation laws exist and therefore the statistical mechanics fails. On the other hand, the propagation of the energy is unbounded for

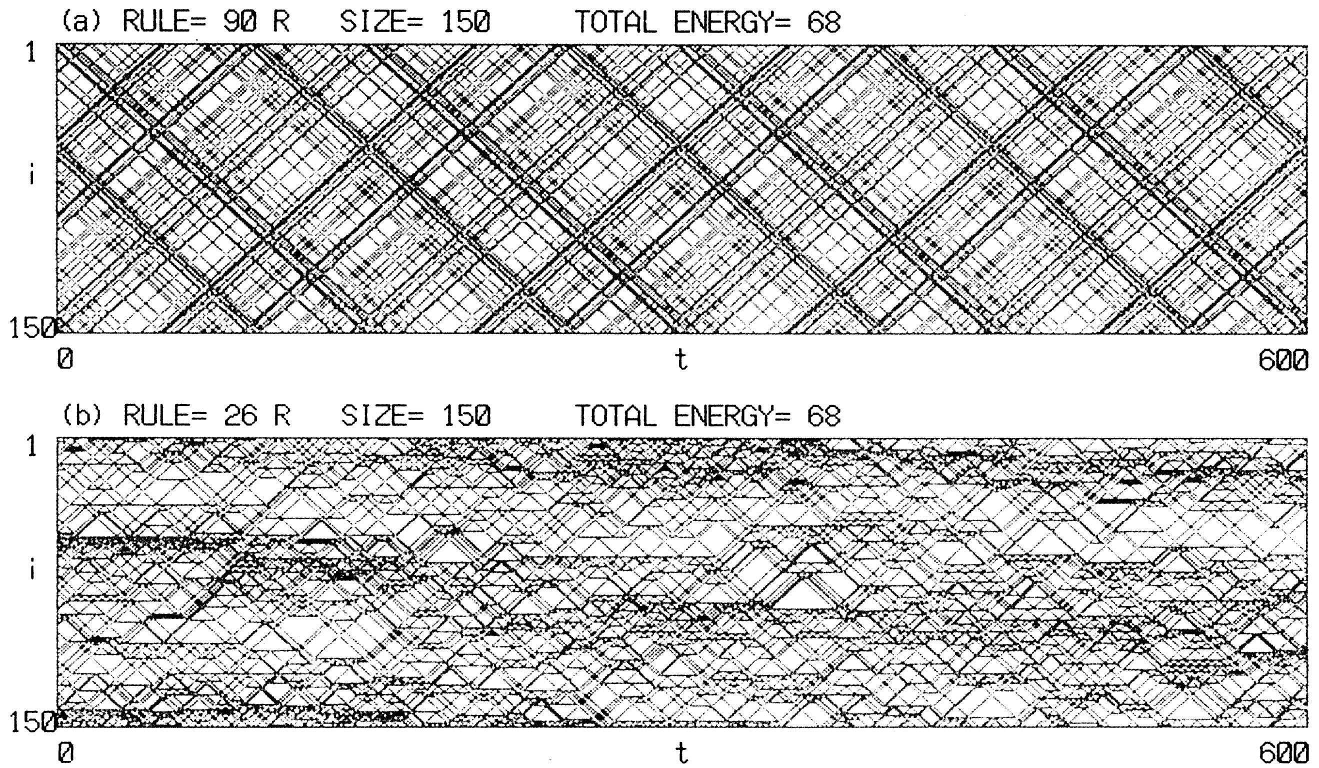

FIG. 1. Time-evolution pattern of the energy given by Eq. (4) for rules (a) $90R$ and (b) $26R$. The space-time point (i,t) is dotted by blue when $F^t_{i,i+1}=1$ and by red when $F^t_{i,i+1}=2$. Undotted points mean that $F=0$ there. The initial conditions are the same for both figures.

rules $90R$ and $26R$, as is shown in Figs. 1(a) and 1(b), respectively.

For rule $90R$, each energy "quantum" moves with a fixed velocity ± 1, which is not affected by other quanta. Thus one can identify rule $90R$ with the ideal gas in which the velocities of constituents are ± 1. As was stated in the beginning, the ideal gas has been proved to be ergodic (in fact Bernoulli) in the thermodynamic limit. Consequently the canonical distribution should be satisfied for rule $90R$ in the same limit, where the number of iterations T has to be less than the cycle length of orbits. For rule $90R$ with N sites, the cycle length being at most N (when N is even) or $2N$ (when N is odd), the limit must be such that $N \geqq T \to \infty$. Figure 2 shows the result of the simulations under the condition that $N=T$. As the system size N becomes large, the canonical distribution becomes precise and applicable for a wide range of the energy of the subsystem. This is a direct consequence of the central-limit theorem.

On the other hand, for rule $26R$, the cycle length is typically of order 2^N. Then I can take the number of iterations much larger than the system size. Since the number of total configurations is 4^N, the finite system is not ergodic. Although no known theorem corresponds to this case, the canonical distribution is well satisfied.

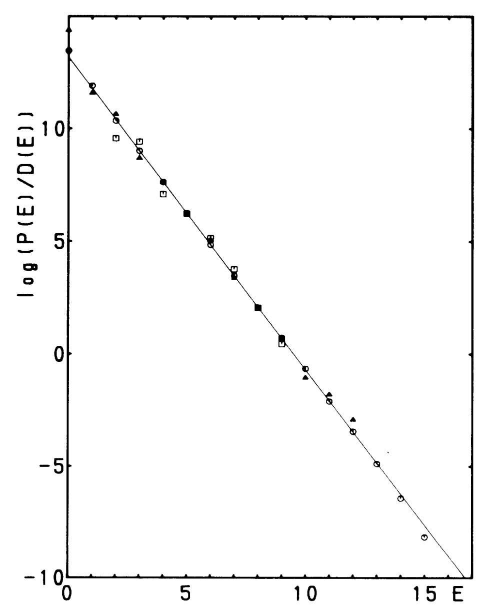

FIG. 2. Plot of $\ln[P(E)/D(E)]$ vs subsystem's energy E for rule $90R$ and the energy (4). Simulations were carried out for three systems with sizes 100 (squares), 2000 (triangles), and 50000 (circles). The size of the subsystem is $n=14$. The solid line was obtained by a least-squares fit for the last case.

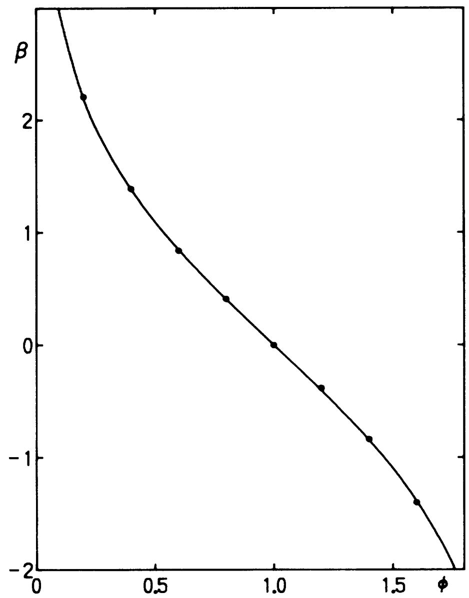

FIG. 3. Comparison between numerically obtained inverse temperature and the analytic β-ϕ relation for rule 26R. Simulations were carried out for systems with size 10^3. For each value of energy density ϕ, 5×10^6 iterations were made.

Namely, $\ln[P(E)/D(E)]$ is proportional to E and the slope $-\beta$ agrees very well with the result of the statistical mechanics, as shown in Fig. 3. For other type-2 ERCA, similar results were also observed.

For a dynamical system to realize statistical mechanics, its subsystem has to forget the memory of the initial condition. In ERCA, the capability of propagation ensures it. For example, it is done in rule 90R by the traveling motion of the initial configuration. Since it returns in time N for the finite system with N sites, I had to take the number of iterations T less than N to see the behavior of the infinite system. On the other hand, the memory is lost by diffusionlike motion through collisions in rule 26R. Consequently T could be taken much larger than N in that case, and then high precision was achieved for relatively small N. This is due to not only the central-limit theorem but also the spontaneous production of stochasticity. The difference between these two rules is their effect on other thermodynamic behaviors. In fact, a temperature gradient can be supported in rule 26R, but not in rule 90R. This and other considerations, in addition to more details on the present examples and other cases, will appear elsewhere.[11]

In conclusion, I have demonstrated that reversible cellular automata yield the canonical distribution function in terms of an additive conserved quantity if it is propagative. I would like to stress that the present models are generally nonergodic in finite systems. The realization of the canonical distribution is connected with the ergodicity of infinite systems.

I thank Y. Takahashi, T. Izuyama, T. Konishi, T. Ikegami, S. Shinomoto, K. Hida, Y. Iba, and K. Kaneko for fruitful discussions and comments, and M. Wadati for a critical reading of the manuscript. This work is partially supported by the Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture of Japan. I am indebted to the Japan Society for the Promotion of Science for financial support.

[1]V. I. Arnol'd, Russian Math. Surveys **18**, 85 (1964).

[2]O. E. Lanford, III, in *Dynamical Systems, Theory and Applications,* edited by J. Moser, Lecture Notes in Physics, Vol. 38 (Springer-Verlag, Berlin, 1975); S. Goldstein, J. L. Lebowitz, and M. Aizenman, *ibid.*; I. P. Cornfeld, S. V. Fomin, and Ya G. Sinai, *Ergodic Theory* (Springer-Verlag, New York, 1982).

[3]O. E. Lanford, III, and J. L. Lebowitz, in Ref. 2.

[4]G. Vichniac, Physica (Utrecht) **10D**, 117 (1984); G. Vichniac, in *Disordered Systems and Biological Organization,* edited by B. Bienenstock, F. Fogelman Soulie, and G. Weisbuch (Springer-Verlag, Berlin, 1986); K. Kaneko, to be published.

[5]Y. Pomeau, J. Phys. A **17**, L415 (1984).

[6]M. Creutz, Ann. Phys. (N.Y.) **67**, 62 (1986).

[7]J. Hardy, O. de Pazzis, and Y. Pomeau, Phys. Rev. A **13**, 1949 (1976); U. Frisch, B. Hasslacher, and Y. Pomeau, Phys. Rev. Lett. **56**, 1505 (1986).

[8]D. d'Humieres and P. Lallemand, Physica (Utrecht) **140A**, 326 (1986).

[9]S. Wolfman, Rev. Mod. Phys. **55**, 601 (1983).

[10]N. Margolus, Physica (Utrecht) **10D**, 81 (1984).

[11]S. Takesue, to be published.

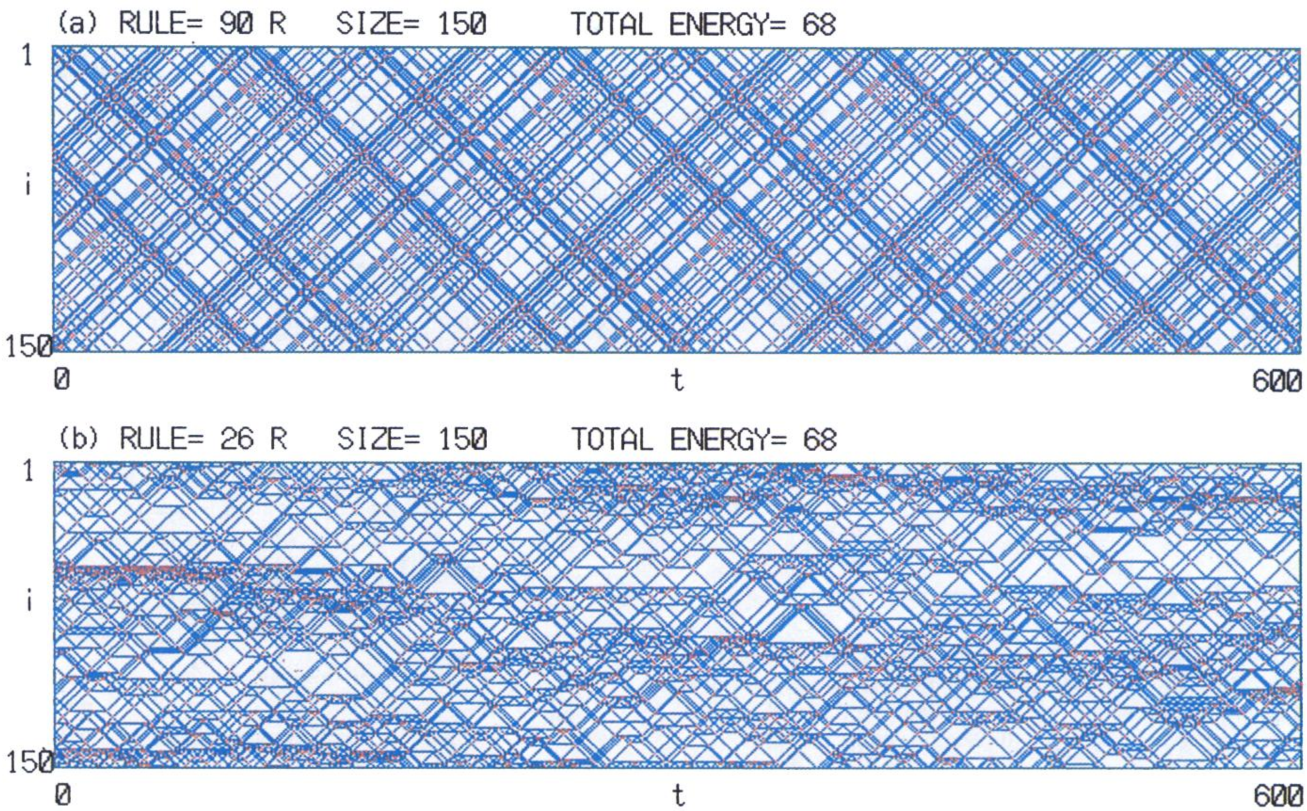

FIG. 1. Time-evolution pattern of the energy given by Eq. (4) for rules (a) $90R$ and (b) $26R$. The space-time point (i,t) is dotted by blue when $F^{t}_{i,i+1}=1$ and by red when $F^{t}_{i,i+1}=2$. Undotted points mean that $F=0$ there. The initial conditions are the same for both figures.