New mechanism for deterministic diffusion

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We show that some of the deterministic one-dimensional cellular automata studied recently by Wolfram exhibit a kind of spontaneous symmetry breaking. The associated kinks (Bloch walls) perform annihilating diffusive walks for large times.

The appearance of stochastic motion in strictly deterministic evolution laws is a phenomenon which has attracted ever increasing attention during the last years. In particular, several mechanisms are by now known which even lead to random-walk–like behavior.[1,2]

In the present note, we shall present a new mechanism, occurring in some of the one-dimensional cellular automata studied recently by Wolfram.[3]

These automata are one-dimensional lattice models, with two states per lattice point ($S_i = 0, 1$), and with discrete time evolution depending on a three-site neighborhood. Models of similar type have been proposed to apply to numerous phenomena, ranging from pattern formation in biological and chemical systems and in crystal growth to the formation of galaxies. Other applications appear in number theory and computer games (the "game of life" of Conway), and as general-purpose computers. References may be found in Ref. 3.

The first model we shall deal with (other ones will be discussed below) is characterized by

$$S_i(t+1) = \begin{cases} 1 & \text{if } (S_{i-1}(t), S_i(t), S_{i+1}(t)) = (0,0,1) \text{ or } (1,0,0) \\ 0 & \text{otherwise} . \end{cases} \quad (1)$$

Here, the index i runs over all integers. In the notation of Ref. 3, this is rule "18," run on an infinite lattice; part of a pattern created in this way from a random start is shown in Fig. 1. The indexing used in Ref. 3 (and in the present paper) is as follows: Write all eight possible states of a three-site neighborhood in a row, in the order given below; write the new state of the center site in the row below; and interpret the obtained series of eight digits as the binary representation of the index of the rule. For rule 18, e.g., this looks as follows:

$$\frac{111}{0}\ \frac{110}{0}\ \frac{101}{0}\ \frac{100}{1}\ \frac{011}{0}\ \frac{010}{0}\ \frac{001}{1}\ \frac{000}{0}$$

$$\rightarrow (00010010)_2 = 18 .$$

The crucial observation of the present paper is that there exist two sets of "ordered" states, which do not mix with each other during evolution. Set I comprises states where

$$S_i(t) = 0 \quad (2)$$

for i even and t even, and for i odd and t odd. Set II is characterized by

$$S_i(t) = 0$$

for i odd and t even, and for i even and t odd.

Consider now an initial state which is in set I for $i < 0$, and in set II for $i \geq 0$. Otherwise, the initial state is supposed to be random. The region around $i = 0$ is then similar to a kink (or Bloch wall) in the Ising model. As in that case, it cannot vanish (except by annihilation with an antikink as discussed below). However, it can move. In Fig. 1, there are three kinks at the beginning. While two of them annihilate later, the third seems to make a random walk.

In a kink-free region, the evolution on the nonempty sublattice is according to the "linear" rule 90. For that rule, the evolution is well understood.[3] It is sensitively dependent on initial conditions in the sense that any localized perturbation spreads with velocity $v = \Delta i / \Delta t = 1$. Thus, the motion of a single kink is influenced by a region increasing linearly with t, with unit velocity. With each time step, its position is shifted left or right, depending on the (random) initial state of the site at the edge of this "light cone." This should result in a random walk with diffusion constant $D = \frac{1}{2}$.

In order to test this numerically, I have performed the following Monte Carlo calculations: with the use of multispin coding as described in Ref. 3, I constructed a lattice of

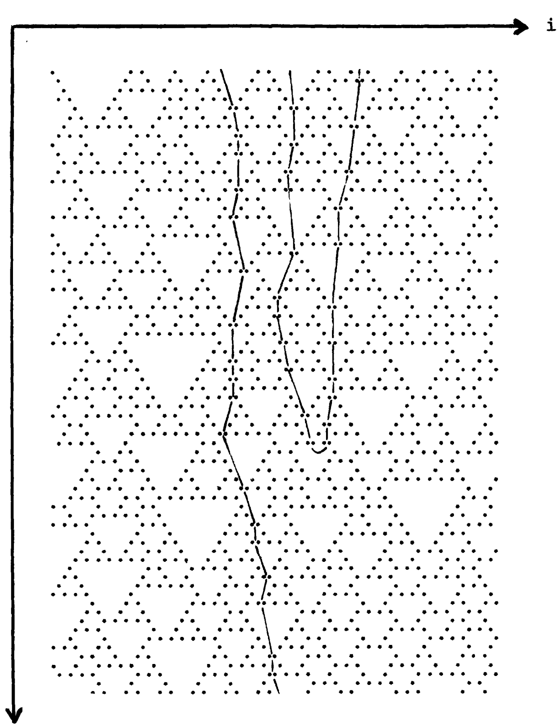

FIG. 1. Part of a pattern created from a random start. For clarity, the kinks are indicated by lines.

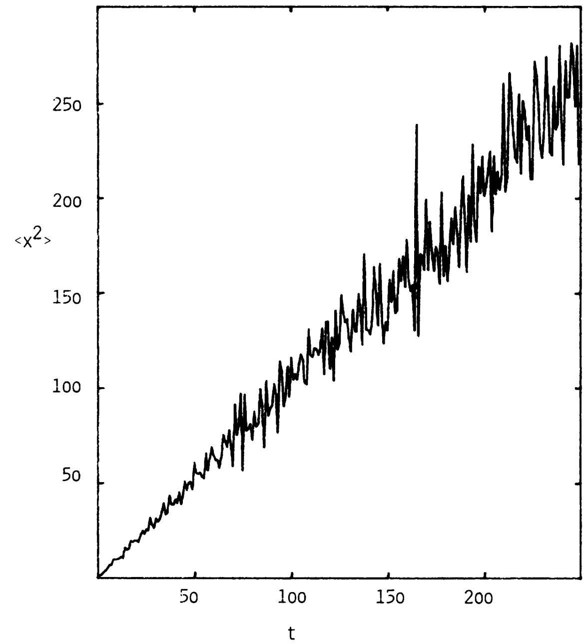

FIG. 2. Average distance $\langle x^2 \rangle$ of occupied pairs from the original kink position vs t. Averaged over 500 kinks originally at $i = 0, 120, 240, \ldots$.

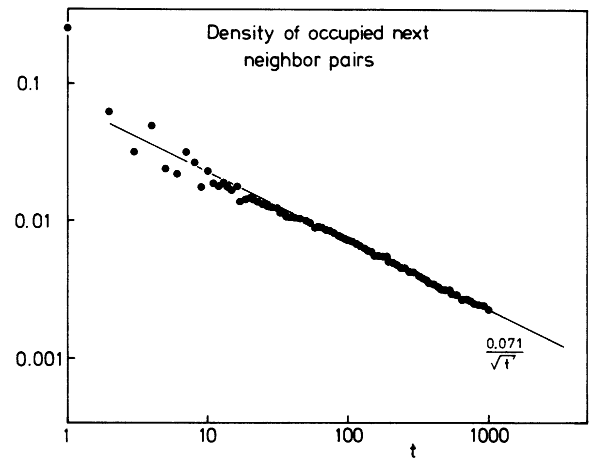

FIG. 3. Average density of occupied pairs after random start (60 000 sites). For large t, values averaged over t are plotted in order to suppress fluctuations.

60 000 sites (with periodic boundary conditions) (1000 words on a Control Data Corporation Cyber 170/720 computer). For the first 120 sites (2 words), the initial configuration was from set I, for the next 120 sites from set II, then again from set I, etc. The motion of the 500 kinks thus created was observed during 300 iterations, by observing occupied neighboring sites $[(S_i, S_{i+1}) = (1,1)]$. The average square distance $\langle x^2 \rangle$ of such pairs from the original position of the corresponding kink is shown in Fig. 2. We see that indeed $\langle x^2 \rangle \approx 2Dt$, with a diffusion coefficient $D = 0.51 \pm 0.01$. We also found from this run that each kink leads to 0.257 ± 0.005 occupied pairs, compared to $\frac{1}{4}$ occupied pairs expected theoretically.

An independent verification of the above conjecture is obtained by starting with a completely random initial configuration. If the kinks move diffusively, their average density will decrease due to recombinations as[4]

$$n_{\text{kink}} \approx \frac{1}{\sqrt{8\pi D t}} \quad \text{for } t \to \infty \; . \tag{3}$$

[In Ref. 4, this was only shown for a particular model with $D = \frac{1}{2}$. The more general Eq. (3) follows from scaling arguments.] The average number of occupied next-neighbor sites versus t, for a lattice with 60 000 sites, is shown in Fig. 3. Using the number of occupied pairs per kink quoted above, we obtain from these data $D = 0.52 \pm 0.02$, in agreement with the above value.

Equation (3) has an interesting consequence for the ergodic behavior. Starting from any random initial configuration, the density of kinks goes to zero with $t \to \infty$, showing that the system remains locally in one of the two states I or II, for increasingly long times. Although this is very reminiscent of spontaneous symmetry breaking, it does not imply nonmixing behavior: for any large time t, there is a $t' > t$ (with probability 1) such that a kink passes through a given i at time t', corresponding to a "tunneling" between the two local states.

For other one-dimensional automata studied in Ref. 3, one finds similar results. First, rules 146 and 182 (for rule 182, one has to exchange S_i with $1 - S_i$, in order to recover the same behavior) lead to the same stochastic long-time behavior as rule 18.

Second, rule 126 can be mapped onto rule 18 by the following procedure: represent any pair $(S_i, S_{i+1}) = (0,1)$ or (1,0) by $\sigma_i = 1$, and any pair $(S_i, S_{i+1}) = (0,0)$ or (1,1) by $\sigma_i = 0$. Evolution of $\{S_i\}$ under rule 126 leads then to evolution of $\{\sigma_i\}$ under rule 18. Pairs $(\sigma_i, \sigma_j) = (1,1)$ indicating a kink in rule 18 correspond thus to $(S_i, S_{i+1}, S_{i+2}) = (0,1,0)$ or (1,0,1) in rule 126.

Finally, rule 122 leads to the same stochastic long-time behavior as rule 126. I might add that in the "ordered" states, the evolution of all above automata is equivalent to the linear rule[3] 90. As a consequence, the asymptotic density of occupied sites is $\frac{1}{4}$ for rules 18, 146, 122, and 126, while it is $\frac{3}{4}$ for rule 182.

Thus we see that all "complex" rules studied in Ref. 3 lead to qualitatively the same long-time behavior, except for rule 22. For this rule, there are (at least) four different sets of ordered states, corresponding to $S_i(t) = 0$ for all even/odd i and all even/odd t. In contrast to the ordered states of rule 18, these states are however unstable: after implanting a kink in an otherwise ordered state, the kink widens without limit, leaving behind it a seemingly disordered state.

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