Short Communication¹

Energy Transport in a Cellular Automaton

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Energy transport in the deterministic Q2R cellular automaton is studied. Two different types of transport processes are found: a diffusion type and a very efficient transport on "highways." The dependence of both types on the energy is investigated.

KEY WORDS: Energy transport; Ising model; cellular automata; Q2R dynamics.

1. INTRODUCTION

Cellular automata have been used to describe a variety of physical phenomena.^(1,2) Specifically, the cellular automaton Q2R³ has been proposed^(4,5) to simulate the thermodynamics of the Ising model. Being a deterministic automaton, Q2R has an unusual dynamics and at low energies a rich structure of clusters of finite periods.⁽⁶⁾ Its energy is strictly conserved.

In this paper we study the transport of energy through a cooperative system, such as the Ising model, putting special emphasis on the behavior close to the critical point. For this purpose Q2R seems particularly suited because it conserves energy and because of its fast implementation on vector computers.⁽⁵⁾ Energy transport in the Ising model has already been discussed, using other types of microcanonical dynamics⁽⁷⁾; we will see that the deterministic nature of Q2R is responsible for a novel kind of transport.

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We consider a square lattice having an Ising spin $\sigma_j = \pm 1$ on each site. Randomly a configuration of a given energy $E = -\sum_{nn} \sigma_j \sigma_i$ is chosen as initial configuration at t = 0. Then at each time unit t the Q2R rule is applied. This rule consists of two steps: the lattice is divided into two interpenetrating sublattices A and B. At the first step each spin of A is flipped if the sum of the spins of its four nearest neighbors (which lie on sublattice B) is zero. At the second step each spin of B is flipped if the sum of the spins of its four nearest neighbors is zero. In this way the energy is conserved for each site. Depending on the value of E, the system will envolve into a situation of finite spontaneous magnetization or not, the critical energy being given by $E_c = -\sqrt{2}$. Since the simulation is microcanonical, the temperature does not appear directly. It could be calculated via exchange probabilities, but we will not do so, but rather express everything in terms of energies.

In order to study energy transport, we consider a finite system of size $N_h \times N_v$ (see Fig. 1) with periodic boundary conditions in the horizontal direction and boundaries of fixed energies E_1 on top and E_2 at the bottom. The energy E on top (or bottom) is fixed by randomly choosing a fraction $(E+2) N_h/4$ of the outgoing vertical bonds to be "frustrated," i.e., to have energy 1, and the rest to have energy -1. During the simulation of one sample the location of the frustrated and nonfrustated bonds is kept fixed. This is assured by furnishing (if the bond is frustrated) or extracting (if the bond is nonfrustrated) an energy of unity each time a site on the top (or bottom) line is flipped. So, at each time step an energy ΔE_1 (ΔE_2) is needed at the top (and bottom) lines in order to maintain the status quo. If, after



Fig. 1. Sketch of the lattice. Frustated bonds on the top and bottom are marked by wiggles. In this case $N_h = 13$, $N_v = 5$, $E_1 = -10/13$, and $E_2 = -2/13$, so that the energy flux goes from bottom to top.

some equilibration time, $\Delta E_2 = -\Delta E_1 = Q$, one has a stationary state of flux Q. An energy transport coefficient κ can then be defined through

$$\kappa(E) = Q/N_h \, dE \tag{1}$$

for $E_1 = E$ and $E_2 = E + dE$.

We have calculated $\kappa(E)$ through a numerical simulation. The results are presented in the next section and discussed in Section 3.

2. METHOD AND RESULTS

We have simulated the above model on a Cray-XMP using a highly vectorized algorithm.⁽⁵⁾ We fixed $N_h = 128$ and varied N_v to study finitesize effects. For each sample, t_{eq} time units were thrown away to reach equilibrium out of a total of t_t time units. For each energy an average was made over M samples, i.e., M independent initial configurations were considered. Totally we used about 10 hr of computer time. We used dE = 0.05 in Eq. (1) and ensured, by also looking at dE = 0.2, 0.1, and 0.025, that our values are independent of dE.

To our surprise, we found two fundamentally different processes contributing to the energy transport: "diffusion" and "highways." In the first process, which is the common one, energy diffuses in an apparently stochastic way in both senses and Q_d is given by the difference of energy that diffuses from bottom to top and the energy that diffuses in the opposite sense. Highways, on the contrary, are structures unique to our deterministic automaton, and are periodic in time and space and transport energy in a highly effective way (one energy unit per time unit). An example for such an highway is given in Fig. 2. These structures do appear after some equilibration time (up to several hundred steps for $N_v = 20$) and constitute some kind of ordered stationary state, since they are domain walls separating regions of plus and minus spins.



Fig. 2. Example of a highway for $N_v = 4$. The period of this structure is two. At each time unit, one energy unit goes from top to bottom. Shown for each time unit are the two individual steps (update of sublattice A and update of sublattice B). The sublattice B is represented by circles and the flux of energy is indicated by the arrows.



Fig. 3. Energy transport coefficient κ_d due to diffusion as a function of energy; $N_v = 20$, $t_t = 6000-12,000, t_{eq} \approx t_0/2$, and statistics M = 200-2000.

The energy transport coefficient κ_d due to diffusion is only finite in the disordered region $E_c < E < 0$, i.e., $T_c < T < \infty$, and goes to zero when one approaches the critical point. In Fig. 3 we see the behavior of κ_d . It seems that $\kappa_d \approx A(E - E_c)$. This behavior qualitatively coincides with the behavior found using other types of Ising dynamics.⁽⁷⁾ However, in the ordered phase our conductivity is vanishing.

The energy transport due to highways strongly depends on the probability f of building such an highway: f is the number of highways/ N_h . We obtained the number of highways by monitoring along the top and bottom lines the energy flux for each site and thus identifying the two end points of each highway. The dependence of f on energy and system size N_v is shown in Fig. 4. We see that there is a maximum number of highways at energies of about -1.0, i.e., above E_c . This maximum is a consequence of two competing effects: at too high energies it is not possible to stabilize large, ordered domains walls separating regions of plus and minus spins that are the highways, and at too low energies the system is not soft enough to allow for a large collective modification of spins that is necessary



Fig. 4. (a) Fraction f of highways as a function of energy for $N_v = 20$. (b) Log-log plot of f against N_v for E = -1.3. For small systems the statistics is M = 60,000; for N_v the parameters are the same as in Fig. 3.

to build a highway. We do not think that the curve in Fig. 4a becomes singular in the thermodynamic limit at some value of E, but we cannot exclude this possibility. The dependence of f of the system size as shown in Fig. 4b suggests that highways are a finite-size effect and disappear in the infinite system with a power law of the system size. This is not astonishing, since in larger systems one has to construct larger highways, which is more difficult.

The energy transported by one highway per time unit is, on the average, of order unity. For high energies it is a little smaller, since then highways also appear transporting energy in the opposite sense. From Figs. 3 and 4 one sees that the contributions to the energy transport due to diffusion and due to highways are of the same order for the system sizes considered in this work. It is interesting to remark that both quantities have strong fluctuations, but of different kind. Diffusion fluctuates enormously in time, and large equilibration times are required to obtain the correct value of the diffusion transport. Highways do not require long equilibration time, but fluctuate very much from sample to sample, and therefore large statistics are needed to get meaningful results.

3. CONCLUSION

We have investigated the nature of energy transport in an Ising model using the Q2R automaton dynamics. Contrary to some previous work⁽⁷⁾ using a different dynamics, we only found energy transport in the disordered phase. In addition to the usual diffusionlike contribution, which vanishes linearly at the critical point, we also found ordered structures of the stationary state, which we call highways, and which transport energy extremely effectively. These highways are important in finite systems.

Two possible physical situations come close to the scenario that we found here. One is transport in a granular medium, where there is also a slow diffusion process through the grains and a fast mobility along the grain boundaries. The other is heat transport in a fluid, where in addition to diffusion convection can also appear, which is represented by ordered structures of the stationary state that are spontaneously formed in the temperature gradient and in this sense have some similarity to our highways.

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