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COMMENT

Domain growth in two-dimensional Metropolis cellular automata

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Abstract. The ferromagnetic 2D Ising model with Metropolis spin-flip dynamics is investigated by computer simulation using checkerboard-type updating. The system is quenched from a high temperature disordered state to a low temperature one at $T \ll T_c$. Domain growth is found to follow dynamic scaling with the value of the domain growth dynamic exponent $Z_{dg} = 1$ in some range of time limited by the size of the system.

In a previous article (Menyhard 1990) the cellular automata (CA) versions of the Glauber (Glauber 1963) and Metropolis (Metropolis *et al* 1953) kinetic Ising models with checkerboard updating have been compared in one dimension. We have found for the Metropolis CA model, as a consequence of the linear law of motion of kinks and antikinks (with velocities $v = \pm 1$ in the case investigated), critical and domain growth dynamical exponents $Z_{cr} = Z_{dg} = 1$, in contrast to the most common Z_{cr}, $Z_{dg} = 2$ behaviour occurring in the case of diffusive kink motion (see, e.g., Kawasaki 1972). It has also been pointed out that the Metropolis CA with its faster relaxation to equilibrium provides an algorithm superior to usual Monte Carlo ones.

The question of similar behaviour in higher dimensions has also been raised there but not investigated. Nevertheless, in an earlier paper by Viñals and Gunton (1986) some results have been reported for the 2D Ising model under the conditions of deep quench below the ferromagnetic transition point. These authors, using the Metropolis CA kinetics, made computer simulation of the $k = 0$ component of the non-equilibrium dynamical structure factor $S(k, t)$ and reported a quicker than power law dependence in time.

In this comment we want to bring evidence of the presence of the linear law of motion also in 2D domain growth kinetics induced—under the conditions of deep quench—by the Metropolis spin-flip dynamics applied with checkerboard updating. Due to the faster relaxation to equilibrium as compared to, e.g., Glauber-type domain growth, the time interval in which scaling prevails is rather limited by the finiteness of lattice size.

We consider the ferromagnetic Ising model in a square lattice of size L with Hamiltonian

$$H(\{s_i\}) = \frac{-J}{kT} \sum_{i,j} s_i s_j \qquad (1)$$

where the sum extends over the four nearest neighbours. $s_i = \pm 1$ and $\{s_i\}$ denote the states of all spins. The dynamics of the model is given by a stochastic interaction with the heat bath. The Metrolis rule (Metropolis *et al* 1953) for the single spin-flip transition rate at site i is given as

$$W_i = \min\{1, e^{-\Delta H}\} \tag{2}$$

where $\Delta H = (2J/kT)s_i \Sigma_{nn} s_j$ is the energy needed for the flip; the sum runs over the four nearest neighbours of spin s_i. This rule is applied at the temperature $T \ll T_c$ of the quench after starting from a disordered situation ($T = \infty$). Domain formation and growth takes place until equilibrium is reached. Checkerboard updating (Vichniac 1984, Pomeau 1984) ensures that the equilibrium state will be a ferromagnetic Ising one.

To characterize the time development of domain growth we have investigated two quantities: the ferromagnetic, $k = 0$, peak of the structure factor which is the non-equilibrium mean square of the magnetization density ($N = L^2$)

$$S(0, t) = N\langle M^2\rangle(t) = N\left\langle\left[(1/N)\sum_i s_i\right]^2\right\rangle \tag{3}$$

and the average energy density

$$E(t) = \left\langle(-J/kTN)\sum_{i,j} s_i s_j\right\rangle. \tag{4}$$

Scaling (see, e.g., Sadiq and Binder 1983) implies the length measures $L(t)$ and $L_1(t)$:

$$[L(t)]^2 = S(0, t) \tag{5}$$

with

$$L(t) \propto t^x \tag{6}$$

and

$$L_1(t) = [1 + (kT/4J)E(t)]^{-1} \tag{7}$$

with

$$L_1(t) \propto t^y. \tag{8}$$

$L_1^{-1}(t)$ is the average perimeter length per unit area.

These two lengths have been measured. The system has been prepared in a completely random state with $\langle M\rangle = 0$ at time step $t = 1$ and rule (2) has been applied from time step $t = 2$ on at a temperature $p = e^{-4J/kT} = 10^{-3}$. ($p_c = 0.1716$ for the 2D Ising ferromagnet). We have investigated lattices of sizes $L = 50$, 100 and 200 and averages over 700 independent runs have been performed. The high number of averages is necessitated by the non-self-averaging nature of the structure factor (Milchev *et al* 1986).

Figure 1 shows $L^2(t)$ while on figure 2 $L_1^{-1}(t)$ is plotted as a function of time on a double logarithmic scale for different values of L. These curves can be fitted with straight lines in the time interval starting after the first few time steps and ranging up to $t_{10} \simeq L/2$. From the respective slopes we get

$$x = 1.0 \pm 0.02 \qquad y = 0.99 \pm 0.02. \tag{9}$$

At t_{10} the system gets very close to its equilibrium arrangement of spins, domain growth is practically terminated and consequently the scaling regime as well. This happens for a lattice of size L^2 if

$$S(0, t_{10}) \propto L^2\langle M^2\rangle_{eq} \propto t_{10}^2 \tag{10}$$

giving $t_{10} \propto L$. Here the observed time dependence, (9), has been made use of.

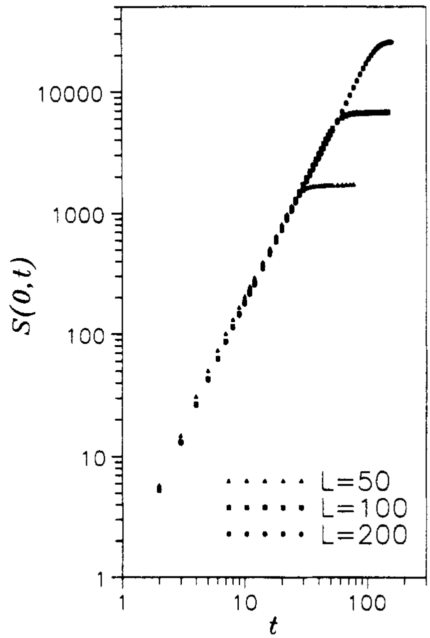

Figure 1. The dynamic structure factor at the ferromagnetic Bragg peak as a function of time for three values of the lattice size L.

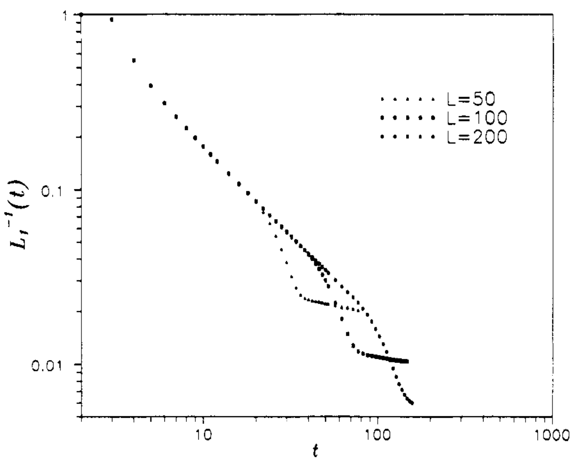

Figure 2. The inverse of the second characteristic length, L_1, proportional to the average domain-wall energy as a function of time for three values of the lattice size L.

It is worth comparing this with the case of the Glauber domain growth dynamics, where from the well known Allen-Cahn (1979) law

$$S(0, t_{10}) \propto L^2 \langle M^2 \rangle_{eq} \propto t_{10} \tag{11}$$

$t_{10} \propto L^2$ follows. Thus, for given L, the scaling regime is much wider in the diffusive case, as can be observed in computer simulations.

The domain growth dynamic universality class of the Metropolis CA model in 2D differs from that of the Glauber dynamics: from the obtained values of x and y, (9), through

$$L(t) \propto \xi(t) \propto t^{1/Z_{dg}} \qquad x = 1/Z_{dg}.$$

$Z_{dg} = 1$ follows, while $Z_{dg} = \frac{1}{2}$ in the Glauber case. From a similar relation applied to $L_1(t)$ the same dynamic exponent results whithin the error of the computer simulation. Thus scaling is valid with one characteristic length in the system manifested by the equality of x and y. This is contrary to the 1D case (Menyhard 1990) where $x = 1$ but $y = \frac{1}{2}$. It is worth mentioning that for both dimensions 1 and 2 the Metropolis rule applied with random sequential updating yields $x = y = \frac{1}{2}$.

Why does Metropolis dynamics (with checkerboard updating) lead to such domain growth properties? Rule (2), considered as a CA rule, has the properties of being (i) deterministic at $T = 0$; (ii) dependent upon the state of the centre cell (outer totalistic in the terminology of Packard and Wolfram (1985)) and (iii) connected with property (ii), non-symmetrical about $\Delta H = 0$; $W_i(\Delta H = 0) = 1$. In 1D (Menyhard 1990), as a consequence of these properties, and the fact that checkerborad updating does not induce randomness in the system (in contrast to usual Monte Carlo), domain walls (kinks or antikinks) move with constant velocity ($v = +1$ or $v = -1$, respectively) making two steps on the lattice in the course of a complete updating procedure leading to the behaviour $\xi = 2t$ for the coherence length of the domain growth problem (quenching to $T = 0$). In 2D domain wall motion is driven by curvature; the coherent movement of larger curved sections of domain walls or of the whole boundary of some domain takes place steadily with maximal velocity in the direction of emptying or filling up some up-spin- or down-spin-phase domain. At some finite L this goes on until there are no longer any larger-scale changes (flat domain walls) and then the scaling regime terminates, the characteristic quantities—as apparent on figure 1 and 2—level off. All these hold only for deep quenches ($p = 0.001$ was chosen in the present computer experiments).

Concerning the equality or non-equality of the exponents in (6) and (8), x and y, the 1D case is pathological and the 2D case is typical. In 1D the only way of changing the domain wall energy, i.e. L_1^{-1}, is the annihilation of a kink with an antikink, the rate of which is determined by the (random) initial state of the lattice (see for references Menyhard 1990). Hence the special dependence upon t of L_1^{-1}, which coincides with the average density of kinks, there. This peculiarity is no longer present in 2D; the vanishing of domains is only one possibility of changing the average perimeter of domain walls. The mechanism for changes in time of the structure factor is not different, in principle, from that of the domain wall energy, thus they scale in the same way.

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