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Unphysical Frozen States in Monte Carlo Simulation of 2D Ising Model

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ABSTRACT

We show that for two-dimensional square Ising systems unphysical frozen states are obtained by just changing the instant of application of periodic boundary conditions during Monte Carlo simulations. The strange behavior is observed up to sample sizes currently used in literature. The anomalous results appear to be associated to the simultaneous use of type writer updating algorithms; they disappears when random access routines are implemented.

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The two-dimensional square Ising model presents a critical temperature T_c above which, in absence of external magnetic field, the magnetization is always zero. Below T_c there is a spontaneous magnetization. Monte Carlo methods have been greatly favored by their application to Ising model in two dimensions because some properties of the later have been obtained exactly [1,2].

However, in Monte Carlo simulation of any system some unavoidable ingredients enter:

- pseudo-random number generators (RNG)
- finite sizes of systems to be simulated
- possible ways to explore the systems

For random number generation more and more sophisticated methods are continuously devised and their goodness for applications permanently tested [3,4,5]. To minimize the effects of boundaries some conditions are usually imposed on them the most popular been probably periodic boundary conditions and helicoidal boundary conditions. Last, the ways to explore the samples more frequently used are the type-writer-like and random access ones.

We demonstrate here that for an appreciable range of system sizes Monte Carlo simulations of the Ising model in two dimensions lead to physically wrong results just by changing the instant of application of periodic boundary conditions (PBC) during runs.

Consider a square Ising system of side size L with PBC to be simulated in a Monte Carlo type writer Metropolis algorithm.

PBC are implemented in the following way: a copy of column *one* is placed side to side with column L, a copy of column L is placed side to side with column *one* the same is done for rows. It is customary to bring up-to-date extra columns and rows while exploring to flip spins (clearly, this is unnecessary if MOD, integer division rest operation, is used to implement periodic boundary conditions). Instead of that we update the extra rows

and columns in a single step after each Monte Carlo step/spin, *i.e.*, after each exploration throughout the whole sample.

There are several reasons that allow and/or advice us to do so, namely, that the number of spins on boundaries is a sub-extensive quantity (there are of the order of $4L$ spins on boundary while the total number is L^2). Another reason (specially in cases where there is a large number of possible transition probabilities making difficult to pre-fabricate a table with them and so slowing down the programs) is of practical character: to avoid the time consuming IF during flipping. It is worth to stress here that any attempt to invalidate this procedure by possible artificially introduced time correlations should be avoided because in usual simulations the copies of row L and of column L are kept constant between one MCS and the next. So if any extra correlation is introduced it is "twice" the normal one and there are no *a priori* elements to wait for radical modifications on simulation outputs.

We have initially employed 32-bit linear congruential algorithms

$$x_n = (a_i x_{n-1})\, MOD\left(2^{31} - 1\right), \tag{1}$$

to generate pseudo random numbers, however, the used type of random number generator is inconsequential as should become clear below. In Eq. (1) the x are random numbers and the a_i are suitable odd numbers.

Figure 1 shows a typical result for the time dependence of magnetization for that kind of simulation. It is a general feature that, independently of the imposed initial conditions the system tends firstly to magnetization values close to the ideal equilibrium ones staying around those values for times that vary with system sizes and with random number generators. After that a "bifurcation" occurs that brings the system to states where nothing change with time.

The appearance of the plot is of a continuous line but actually are single points states for each Monte Carlo step. The two "parallel lines" suggest that there exist states for which each spin changes its orientation in each attempt to flip it. Those configurations

do exist and a snapshot of a typical one is shown in Figure 2. That type of configuration although physically possible is largely improbable, there are of the order of L such different configurations. However if any of them appears in a simulation or is used as initial condition it will never change (actually it becomes its negative) as can be easily tested by mimic a type writer Metropolis updating scheme by hand beginning at the left upper corner of Figure 2.

Figure 3 shows a pattern when "equilibrium" has not yet been reached. The extraordinary patterns are created at the boundaries and gradually extended to the rest of the sample.

In Table 1 the explored ranges of temperatures and the corresponding behaviors are summarized. We have include the $T > T_c$ region as a separate case because for that range of temperatures the magnetization value the simulations tend always to initially, is *zero*, in contrast to what happens when $T < T_c$. For systems sizes below $100x100$ spins the formation of the strange patterns takes a few ten Monte Carlo steps.

Contrary to what could appear at a first reading the more problematic sizes are not too small, they are currently appearing in literature for several Ising-like models[6,7].

It is not possible to look for an explanation in random number generator cycles. The fundamental fact supporting such a statement is that the simulations present the anomalous behavior for a "continuous" range of system sizes and not for some special ones. Furthermore, the unhealthly states are attained long before typical RNG cycles have been completed. The wrong results appears to be related to the simultaneous application of "new" PBC and type writer like updating schemes. The uncommon behavior disappears if random access algorithm are used.

The correctness of the particular instant we choose for application of PBC is strongly supported by two facts: simulations always tend initially to values of magnetization near correct ones and, for greater system sizes (as expected from sub-extensive criteria above) unphysical results tend to disappear.

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FIGURE CAPTIONS

Figure 1.- Typical time dependence of the magnetization. The time units are Monte Carlo Step/spin. The initial magnetization was ∼0,33 and the temperature $T = 2,0 < T_c = 2,269$ (in units where the interaction constant is numerically equal to Boltzmann constant). The arrow points approximately to the equilibrium value of traditional simulations.

Figure 2.- Snapshot of a typical final configuration. The black squares standing for up spins and the white ones for down spins. If used as initial configuration for single spin type writer Metropolis algorithms remains invariable forever. The temperature $T < T_c$.

Figure 3.- Snapshot of the system before attaining a configuration of the type shown in Figure 2. Note that the strange patterns are created at the boundaries. The temperature $T > T_c$ but the final apparence is the same.

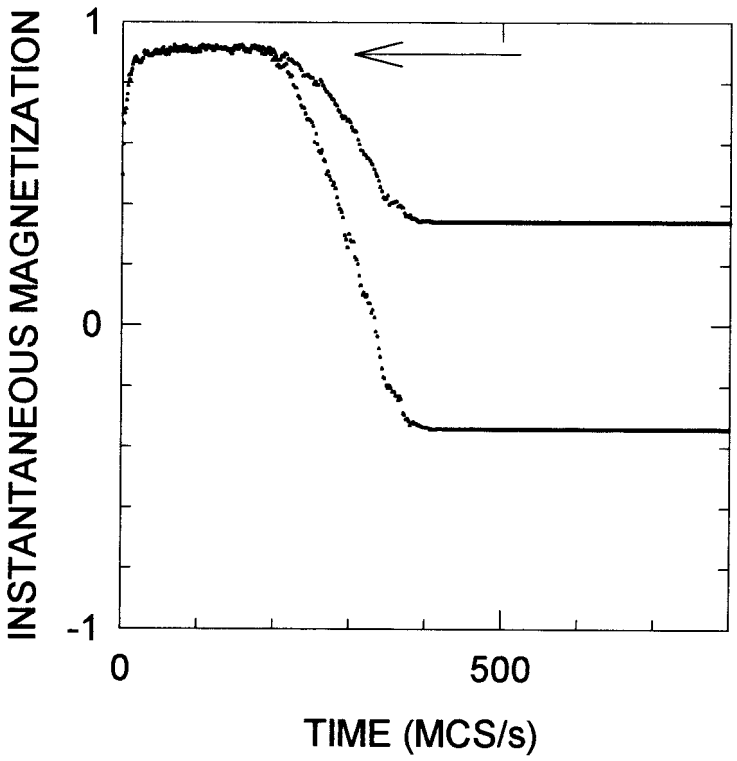

Figure 1

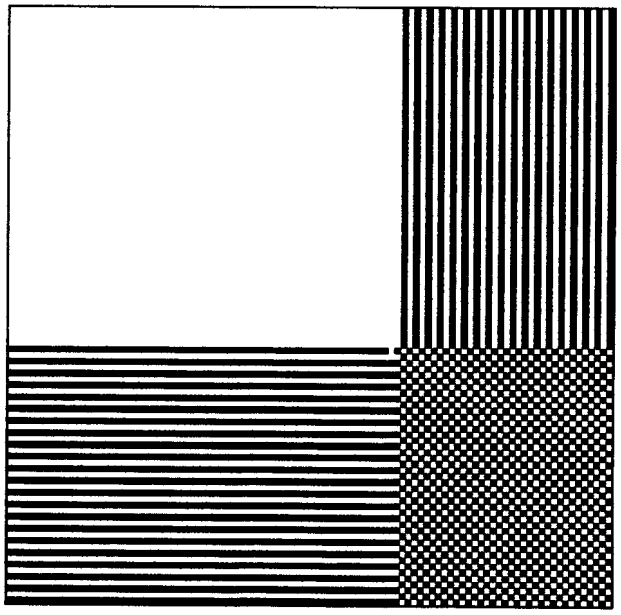

Figure 2

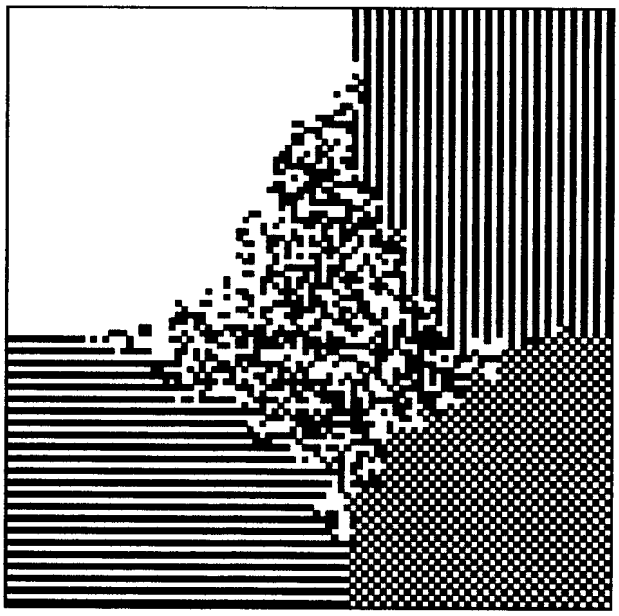

Figure 3

TABLES

TABLE I. Observed behavior in Monte Carlo simulation of 2D Ising systems for different temperature ranges. The instant for application of periodic boundary conditions during runs is not the usual one. We show the $T > T_c$ range as a separate one because on those cases the magnetization always tends initially to the value zero. As bigger systems are the longer the time needed to observe the onset of unphysical patterns.

	$T < 1,5$	$1,5 \leq T < T_c$	$T > T_c$
for any system size	normal	unphysical	unphysical

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