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Abstract: Random number generators based on the congruence method have long range correlations which can severely influence Monte Carlo simulations of lattice theories, especially in critical regions. We investigate the nature of these correlations both theoretically and in test simulations. We propose practical ways to avoid that random number correlations affect the simulation results.

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1. Introduction

It has been recently reported by several authors [1-3] that Monte Carlo (MC) simulations of lattice models in critical regions might be affected by long range correlations in the random number generator (RNG) used. These effects turn out to be strongly dependent on the lattice size and occur typically for large lattices.

An important class of RNG's is based on the congruence method [4]. Many high-speed computers offer RNG's of the type

$$n_{i+1} = an_i \pmod{2^m}; \quad r_{i+1} = n_{i+1} / 2^m \tag{1.1}$$

where a is a fixed odd integer called multiplier, 2^m is called the modulus, the numbers n_i are integers and the actual random number r_i is obtained by dividing n_i by the modulus. The integer n_o is called the seed of a sequence of random numbers.

RNG's of the type (1.1) always have correlations at distances of powers of 2 which are independent of the special multiplier and seed chosen and only depend on the modulus. These correlations are especially dangerous for MC renormalization group calculations [5] that use lattice sizes of powers of 2.

It is easy to find explicit formulas for these correlations. In this paper we investigate their influence on various MC simulations and propose methods to circumvent the problems they cause.

In section 2 we present several MC calculations for a 4-dimensional Z_2 gauge theory and for the 4-dimensional Ising model, where we first encountered the problem that RNG correlations drastically alter the results. These calculations have been performed on a CRAY 1/M computer using RANF as RNG. RANF is generally considered to have good statistical properties. The difference between the "wrong" and the "correct" results was already striking in simulations that used 2^{28} random numbers (the period of RANF is 2^{46}).

In section 3 we show that RNG correlations at distances of powers of 2 are inherent in the congruence method by explicitely deriving correlation formulas.

In section 4 we discuss several tests we made in order to study the influence of RNG correlations on MC simulations in more detail. In particular we find that the Metropolis algorithm is much less sensitive to these correlations than the heat bath algorithm (for Z_2 models).

2. Irregularities in Monte Carlo Simulations

We investigated numerically the 4-dimensional Z_2 gauge theory with matter field [6,7] and found a line of second order phase transitions separating the screening from the free charge regions of the phase diagram of Fig. 1 (the results of these calculations are reported elsewhere [8]). In order to check finite size scaling relations and calculate critical exponents, we measured the link-link susceptibility (the integral over link-link correlations) for $\beta_g=.5$ and lattice sizes L= 4,6,8,12 and 16. We used the heat bath algorithm [9 - 10] which requires one random number per update. So $5L^4$ random numbers are needed for one full sweep (there are L^4 point variables and $4L^4$ link variables in the model). The results for L=16 were completely different from what we expected by extrapolating the results for smaller lattice sizes, as shown in Fig. 2.

Then we performed thermal sweeps [9] (β_h was slowly varied through the critical region, β_g was kept fixed at 0.5) for L= 10,12,14,16,18 and 22. The results for the link expectation value for L= 12,16 and 22 are shown in Fig. 3. The curves for L= 10,14 and 18 are practically the same as for L= 12 and 22. Again L= 16 does not agree with the other results.

For β_g =.6 the thermal sweeps show the same discrepancy between L= 16 and all the other values of L. For $\beta_g \longrightarrow \infty$ the model goes into the 4-dimensional Ising model. The link expectation value becomes the energy density in this limit. Here too thermal sweeps show the same irregular behaviour for L= 16. Note that in the Ising limit only L^4 random numbers are needed for each sweep.

Since successive updates at the same lattice site occur every L^4'th random number we suspected that the RNG has correlations over distances of $16^4 = 2^{16}$ which somehow interact with the correlations occuring in the MC simulation of the model in the critical region. In order to disturb these correlations we omitted after each sweep a certain number of random numbers. The results for L = 16 were drastically changed (for all values of β_g considered) whereas the results for the other values of L remained unchanged. In fig. 2 the new values for L = 16 (the "correct" values) perfectly fit into the series of results obtained for the other lattice sizes. Moreover, the new results were independent of the number n_r of random numbers omitted after each sweep (n_r = 1,2,3,4 or randomly chosen between 1 and 100). In fig. 4 we compare for the 4-dim. Ising model the thermal sweep behaviour of the energy with and without the ommitted numbers. For all values of β_g considered, the correct L = 16 thermal sweep curves practically overlap with those for L = 12 and 22.
The results are shown in fig. 4. The new L = 16 results perfectly fit into the series of results obtained for the other lattice sizes.

3. Correlations in Congruential Random Number Generators

In order to understand the problems caused by RNG's based on the congruence method, we take a closer look at eq. (1.1). We are interested in the subseries

$$n_i^{(k)} := n_{i2^k} \qquad (3.1)$$

which is generated by the relation

$$n_{i+1}^{(k)} := a_k \, n_i^{(k)} \pmod{2^m}$$
$$a_k := a^{2^k} \pmod{2^m} \quad . \tag{3.2}$$

The relevance of such subseries for MC calculations has already been emphasized in [1].

The multiplier a is always chosen to be odd; otherwise $a^m = o \pmod{2^m}$ and the original series would degenerate after m steps. Thus $a^{\ell} \pm 1$ are even numbers for each positive integer ℓ, and either a-1 or a+1 is a multiple of 4. Therefore, using the factorization

$$a^{2^k} - 1 = (a-1) \prod_{l=o}^{k-1} (a^{2^{\ell}} + 1) \tag{3.3}$$

we conclude that $(a^{2^k} - 1)$ is a multiple of 2^{k+2}, and the same holds for $(a_k - 1)$ if $k+2 \leq m$. Furthermore, if $a \pm 1$ is not a multiple of 8, then

$$a_k - 1 = c_k \, 2^{k+2} \tag{3.4}$$

with c_k odd.

In spite of the fact that the number of digits in the binary representation of c_k may be large (for the discussion in section 2 m = 48 and k = 16, so c_k still has 30 digits), the statistical properties of the series (3.1) can be very poor. This fact can be described in terms of the "potency" of a_k [4]. The potency of a_k is defined to be the smallest natural number s with

$$(a_k - 1)^s = 0 \pmod{. \; 2^m} \tag{3.5}$$

For the considerations above, s is the smallest integer larger than or equal to $\frac{m}{k+2}$, hence in the case of m = 48 and k = 16 the potency of a_k is 3. Eq. (3.5) implies the following formula, which relates s + 1 subsequent numbers of the series (3.1):

$$\sum_{j=o}^{s} \binom{s}{j} (-1)^j \, n_{i+j}^{(k)} = 0 \pmod{2^m} \tag{3.6}$$

Thus in our case (m = 48, k = 16, s = 3) 4 subsequent random numbers always fulfil the equation

$$r_{i+3}^{(16)} - 3r_{i+2}^{(16)} + 3r_{i+1}^{(16)} - r_i^{(16)} = 0 \pmod{1} \tag{3.7}$$

In general (see the discussion in ref. [4]) a potency of at least 5 seems to be necessary for the series (3.1) to have good statistical properties.

If $\frac{m}{k+2}$ is only slightly larger than an integer, another type of correlations, relating s subsequent numbers in the series (3.1), becomes important. One has:

$$2.^{m-(s-1)(k+2)} \sum_{j=0}^{s-1} \binom{s-1}{i} \; n_{i+j}^{(k)} = 0 \pmod{2^m} \tag{3.8}$$

In the original series (1.1) there are lots of other correlations related to the discussion above. They can be derived from formulas of the type

$$(a_{k_1} - 1) \ldots (a_{k_2} - 1) = 0 \pmod{2^m} \tag{3.9}$$

with $\sum_{i=1}^{\ell} k_i + 2\ell \geq m$.

All these correlations exist independently of the choice of the multiplier a. In addition, for a given a (for RANF a = 44485709377909) there are other correlations. All of them follow from equations of the form

$$\sum_{i=0}^{n} b_i\, a^i = 0 \pmod{2^m} \qquad (3.10)$$

with integer b_i, and their strength may be estimated by computing the quantity $d = (\sum b_i^2)^{-\frac{1}{2}}$ [4] (larger values of d imply stronger correlations).

4. Numerical tests and conclusions

The detailed mechanism according to which a lattice model reacts to the correlations (3.6) – (3.8) is not yet completely understood. However, the results presented so far suggest that the RNG correlations have a larger impact on a MC simulation when the correlations in MC time [10] are longer. We made the following tests in order to investigate this problem more thoroughly and to get a feeling of what might happen.

First we performed thermal sweeps on the 4-dim. Ising model on a 16^4 lattice (heat bath method), deleting random numbers only after n = 4,6,8 and 16 sweeps. The results were correct for n = 4 (see fig. 4), while for n = 8 and 16 they were wrong (n = 6 was unclear). This is consistent with our observation that the results without omitting random numbers at all differed from the correct ones only for temperatures where the MC time correlation length was of the order of 10 or larger.

Next we investigated the effect of the RNG correlations using the Metropolis algorithm [9-11] (the program generated

one random number per spin update, so the periodicity was the same as before). In this case the MC time correlations are much shorter than for the heat bath method. It turned out that the discrepancy between the correct and the wrong results is roughly ten times smaller than for the heat bath method.

In order to check the period 2^k in a simple model, we simulated the 2-dim. Ising model on a 20 x 20 lattice (heat bath) omitting (2^k-400) random numbers after each sweep. The system turned out to be sensitive to the correlations (3.6)-(3.8) for $k \geq 20$. As in the 4-dim. case the results became correct if additional random numbers were omitted after each sweep. We repeated the 2-dim. calculation on an IBM 3081 using ZPF as RNG (ZPF is of the type (1.1) with m = 31; it is the standard RNG offered by the DESY program library). The results were wrong for $k \geq 14$.

At this stage we have gained some insight into the interplay between RNG correlations at a fixed lattice point and MC time correlations. On the other hand, correlations between different lattice points seem not to contribute to the observed effects. Otherwise the results should have changed when varying the number of random numbers omitted after each sweep. Moreover, permutations of the order in which the lattice sites are updated did not alter the results either.

Presumably this is not the most general case. It is to be expected that in the deep critical region the correlations of the model itself interact with the RNG correlations. In general one would have to check, for each particular algorithm, whether highly correlated points in the (lattice-variable x MC time)-space are updated by correlated random numbers. An empirical check would be the stability of the simulation against changes in lattice size and against omission of different numbers of random numbers. In any case a periodicity of the updating process with a large power of 2 should be avoided.

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Figure captions

Fig. 1 The phase diagram of the 4-dimensional Z_2 gauge theory with matter fields (from [8]).

Fig. 2 Link-link susceptibility in the peak region for various lattice sizes L (from ref. [8]). The "correct" values for L = 16, as opposed to the "wrong" values, were obtained by omitting random numbers after each sweep.

Fig. 3 Thermal sweeps for β_g = .5, with no random numbers omitted.

Fig. 4 Thermal sweeps for the 4-dimensional Ising model with and without omitting random numbers after each sweep.

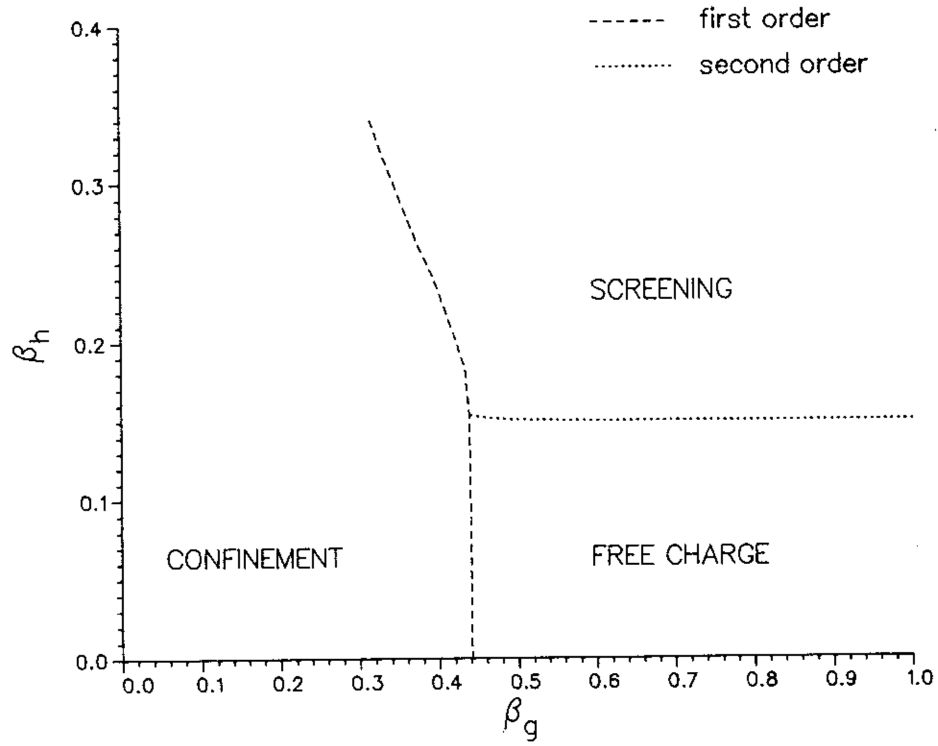
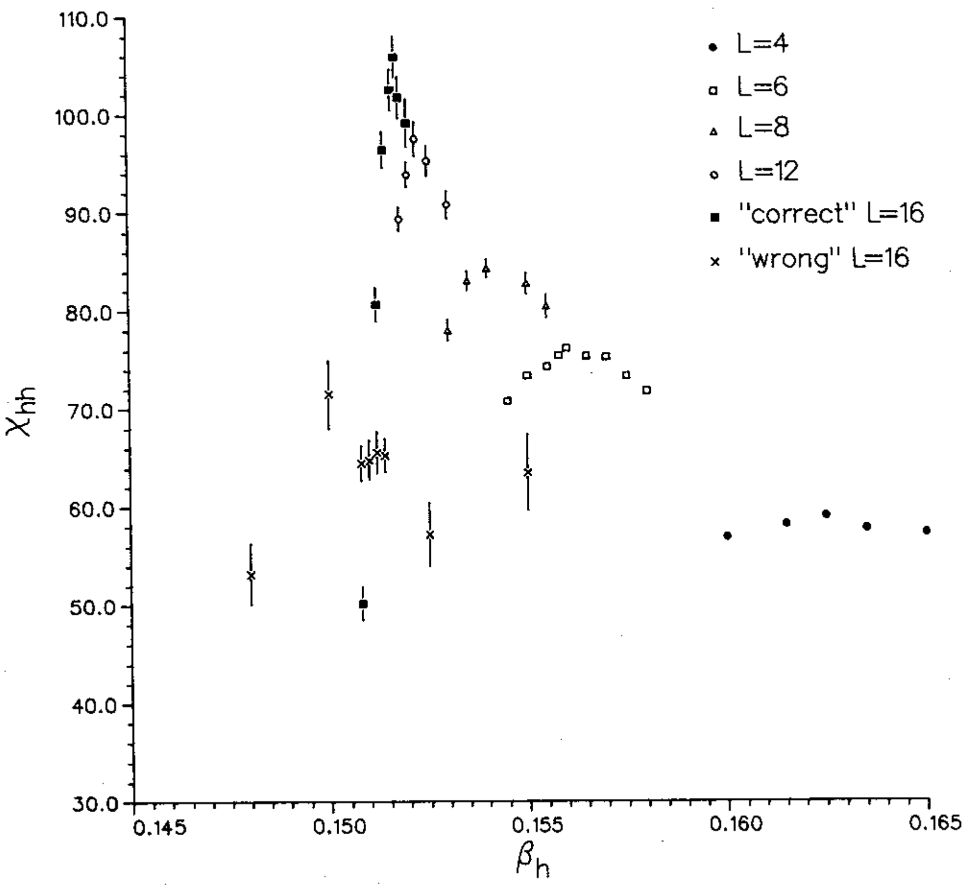


Fig. 1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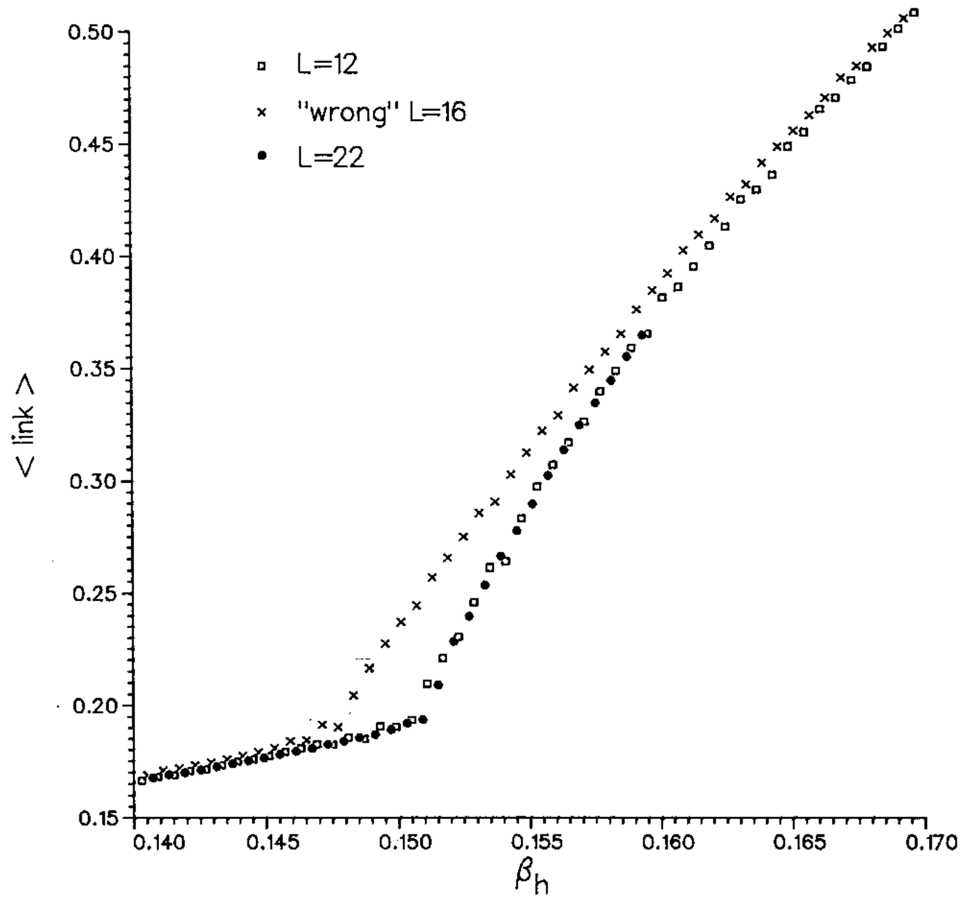
0.155
0.160
0.165
χ_{hh}
β_h

Fig. 2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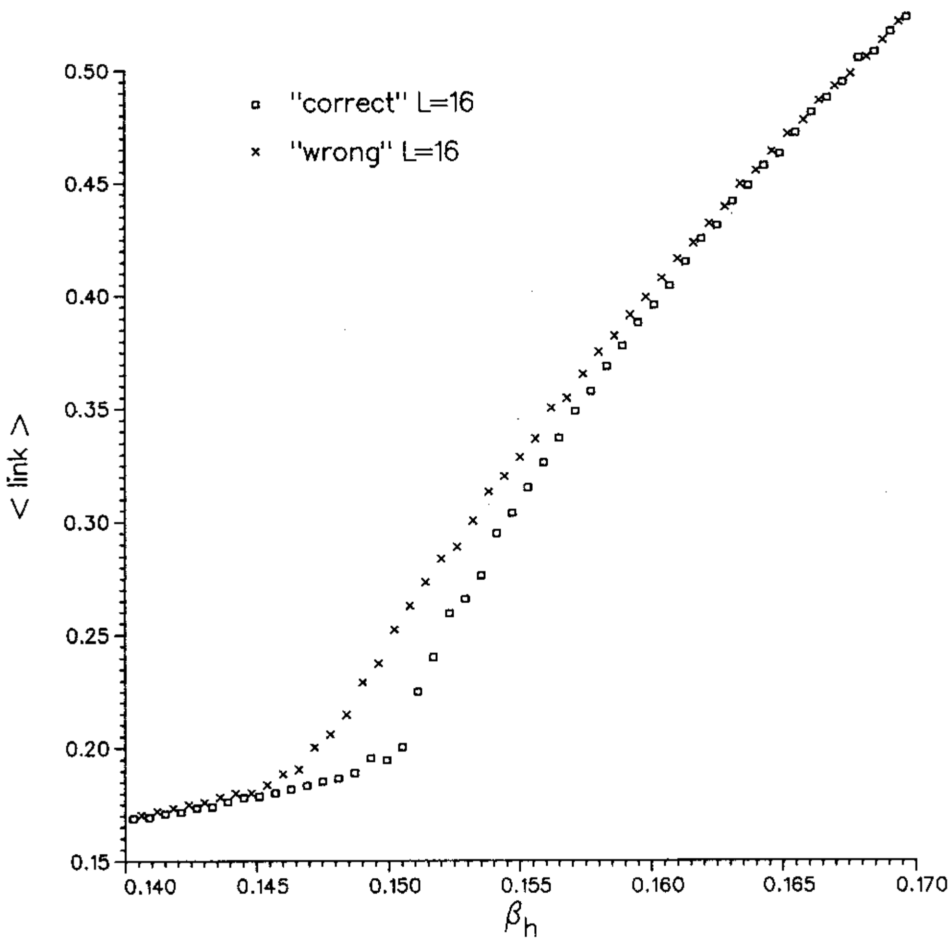
β_h

Fig. 3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0.20
0.15
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0.145
0.150
0.155
0.160
0.165
0.170
β_h

Fig. 4