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Short Communication

Confirmation of Rieger definition of Ising clusters

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Abstract. — A very simple definition of Ising clusters was introduced by Rieger which joins spins with an average individual magnetization opposite to the global magnetization. Involving percolation methods we get very good agreements between the critical temperatures and the percolation thresholds of diluted and undiluted Ising systems in various dimensions.

1. Introduction.

Clusters in the Ising model (energy = $- \sum_{i,j} J S_i S_j$) are usually described by the definition of Coniglio and Klein [1, 2] connecting bonds between parallel spins with probability $w(T) = 1 - \exp(-2J/kT)$. For a better understanding of the geometrical properties of the Ising model various alternative cluster definitions were tested in the recent years [3-6], mostly trying to replace the "external" probability function $w(T)$ by a system inherent quantity measured empirically.

Some of the ansatizes give good approximations of the critical temperature by the percolation threshold, i.e. the first appearance of a spanning cluster, but they fail in reproducing exact agreement (e.g. [6]). We examine the equilibrium properties of a cluster definition which was firstly introduced by Rieger for the determination of non-equilibrium dynamics [7].

Therefore we start simulation with an arbitrary initial spin configuration – we chose the ferromagnetic ground state – at a given temperature and we wait until the Ising system relaxes into the equilibrium state, i.e. the overall average magnetization rests constant in time. Then we calculate the average spin direction of each single spin with respect to an observation interval $I$. Further all spins with a local magnetization opposite to the global, say positive, magnetization, i.e. all spins with

$$< s_i >_I = \frac{1}{I} \sum_{t=1}^{I} s_i < 0$$

(1)
by definition build the Rieger clusters as groups of neighbouring spins with negative local magnetization. To calculate the spanning fraction of these clusters we examined up to 128 samples of each system.

Some attention has to be paid on the examination of Ising systems with small \( L \) approaching \( T_c \) form below, because large statistical fluctuations may appear within the observation interval \( I \). These fluctuations may enable the system to overcome the energy barrier between the equilibrium state of the system and the reversed system which has a negative global magnetization. The dynamics of such “flipping” systems differs of course from the dynamics of the larger systems where fluctuations are small compared with the energy barrier between the two energy minima. Also the cluster definition of “flipping” systems is ambiguous.

Our results confirm that these effects are important for the interpretation of the data for the small systems only. We show further, that this finite size effect can be filtered out, if one uses a rejection method which neglects “flipping” samples.

Above \( T_c \) the energy minimum of the Ising system has zero magnetization and so “flipping” of the system in the described way does not appear, although of cause the global magnetization fluctuates around zero and changes the sign often.

2. Results.

Figure 1 shows the spanning fraction \( R(T) \) for the undiluted Ising model in 3 dimensions with linear size \( L \). \( R(T) \) is the number of samples where a Rieger cluster spans from top to bottom, divided by the total number of samples. For the biggest system examined, \( L = 105 \), the spanning fraction changes from 0 at \( T < T_c \) to a finite value for \( T > T_c \). On the other hand the smaller systems seem to allow percolation of the Rieger clusters with nonzero probability even below \( T_c \).

A comparison of figures 1 and 2 shows that these deviations are mainly caused by the changes of the sign of the global magnetization described above. The data of figure 1 represents all examined samples while figure 2 considers only the samples with a positive magnetization at the end of the observation interval and gives better results for the smaller systems.

For \( L = 105 \) however, no changes in the sign of the magnetization can be observed and so all samples contribute to the spanning fraction of figures 1 and 2.

The simple rejection law of figure 2 makes the results of the \( L = 83 \) system agree with those of the bigger system. For medium size systems the frequency of the changes in magnetization is small and nearly all systems which have a negative magnetization within the observation interval stay into this state for the rest of the interval and therefore are correctly neglected if one examines the global magnetization only at the end of \( I \).

Obviously this selection method is not sufficient for very small systems. For \( L = 41 \) the fluctuation of the global magnetization is much more frequent and so it is nessessary to check explicitly after each time step of the interval that the global magnetization is positive. The number of successful samples which show positive magnetization for the whole interval length of 4000 time steps of course decreases rapidly for small systems if \( T \) approaches \( T_c \), and so many samples have to be neglected. But even for \( L = 41 \) the spanning fraction vanishes for \( T < T_c \) as far as only the “correct” samples are selected.

For \( T > T_c \) figures 1 and 2 show no significant differences. The simple rejection law – check for magnetization at the last time step of \( I \) – only decreases the statistics by neglecting the samples with a negative magnetization by \( 1/2 \). The strict rejection law – check for magnetization at each time step – of cause does not work at all for large enough \( I \), independent of the system size \( L \), because the magnetization fluctuates around zero. But for \( T > T_c \), as stated above, no rejection law at all should be necessary.
Fig. 1. — Spanning fractions in the undiluted Ising model, all samples (dimension $d = 3$, fraction of magnetic sites $p = 1$).

Fig. 2. — Spanning fractions in the undiluted Ising model, selected samples ($d = 3, p = 1$).
Fig. 3. — Spanning fractions in the diluted Ising model, selected samples ($d = 3, p = 0.8$).

Fig. 4. — Spanning fractions in various dimensions, selected samples ($p = 1$).
Fig. 5. — Dependence of spanning fraction on interval length, selected samples \(d = 3, p = 1\).

Considering the correct definition of the Rieger clusters as clusters of spins of local magnetization opposite to the global magnetization and therefore calculating the spanning fraction by considering only those samples that do not change the sign of the global magnetization we can state that the critical temperature of the Ising system and the percolation threshold of the Rieger clusters agree within 0.1 per cent of accuracy for all examined system sizes.

Figures 3 and 4 confirm the Rieger cluster definition for building spanning clusters right at \(T_c\). All the data is based on the simple selection method which neglects samples with a negative global magnetization at the end of the observation interval. The Ising systems in 4, 5 and 6 dimensions as well as the diluted Ising system (we examined \(d = 3\) and 20\% dilution and used Heuer’s [8] \(T_c\) estimate) agree within nearly the same accuracy as the undiluted 3 dimensional Ising model. Of course the statistical fluctuations in the diluted Ising model are slightly bigger, so that the simple rejection law may not work correctly even for the \(L = 83\) system and for figure 4 finite size effects are more important because of the small \(L\) in high dimensions. The Ising system in 2 dimensions does not allow very exact data because the relaxation time of the magnetization is very long and accordingly it is very difficult to reach thermal equilibrium.

Figure 5 shows, that the agreement of the critical temperature and the percolation threshold vanishes if short time periods \(I\) for the determination of the spin magnetizations are considered. With respect to the small system size of \(L = 41\) we use the strict rejection law for figure 5.

On the other hand for very long intervals up to \(I = 50000\) we find no hint for a possible homogeneization of the system – cf. next section – and thus no hint for a corresponding deviation between the threshold and \(T_c\) within the big error bars for the examined small system \((L = 21)\).
3. Conclusions.

The results of the previous section are somewhat surprising especially for the undiluted Ising model because the symmetry of this system – we use helical boundary conditions – should force all spins to get equal local magnetizations in the limiting case of $I \to \infty$. Also even for finite temperatures at and above $T_c$ roughly half of the spins should have a negative magnetization as well as roughly half of the spins point down in each time step. So one should expect that whyever the Rieger definition is correct for small interval length, the validity may vanish for very long $I$. As far as our simulations are concerned such effects could not be observed. On the other hand we see, that the geometrical information of the Rieger clusters needs some time to establish, for the simulations with observation intervals shorter than 1000 time steps do not agree within the same accuracy as the longer intervals. In addition graphical analyses show that the stability of the Rieger clusters is very much larger than that of the classical cluster definition. The decay of the local spin correlations in time seems to be orders of magnitude smaller for the Rieger clusters.

According to this the validity of the Rieger cluster definition with respect to the agreement of the percolation thresholds and the critical temperatures may give new insights into the cluster connection, the cluster stability and the cluster movement.

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