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## Mapping of frustrated spin systems into percolation models and Monte Carlo cluster dynamics

Mario Nicodemi†

Università di Napoli, Dipartimento di Scienze Fisiche, Mostra d'Oltremare Pad. 19, I-80125 Naples, Italy

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**Abstract.** A criterion is introduced to find solutions for the mapping of Ising spin systems into generalized percolation models through the extension of the Kasteleyn–Fortuin technique, and specific application to the 2D triangular fully frustrated Ising model is given. The clusters of generalized percolation, selected according to a general scheme, give the way to implement efficient Monte Carlo (MC) cluster dynamics for frustrated Ising spin systems, and the study of their geometric properties suggests the understanding of MC performances.

The introduction of geometrical and percolation concepts to study unfrustrated and frustrated Ising and Potts models [1, 2] has greatly enhanced both the theoretical understanding of such systems [3–5] and the possibility of implementing fast Monte Carlo (MC) cluster dynamics [6–10]. The importance of developing tools to manipulate and control the geometrical structure of spin clusters and specifically to use it to describe correlation patterns of the system has been pointed out [11, 12]. The comprehension of the relations between clusters and spins, i.e. the knowledge of the structure of ‘physical’ clusters [13], has been usefully exploited in many directions, even if the problem of developing efficient MC dynamics for frustrated and disordered Ising spin systems is still to be successfully faced.

Recently, a general criterion for defining clusters in such systems has been proposed through a mapping of the spin system into generalized percolation models imposing conditions to make the thermodynamical critical behaviour as similar as possible to the geometrical percolative one [12]. This procedure has proved capable of separating clusters whose percolation point may be pushed towards the thermodynamical critical point in the spin system, and whose related MC cluster dynamic shows greatly improved performance in the critical region. The question about the real applicability limits of such a criterion to generate general efficient cluster dynamics and the possibilities of success of its extensions to more complex systems remain open.

This paper is focused on such a problem. After a brief description of the extension to general Ising spin systems of the Kasteleyn and Fortuin mapping equations introduced in [12], in section 1 general criteria to push cluster connectivity toward spin correlation are discussed. In section 2 the problem of actually finding solutions of the mapping equations, and quoted conditions introduced in section 1 to define suitable clusters for MC simulations, is faced and explicit solutions presented in the case of the 2D triangular fully frustrated

† E-mail address: nicodemim@axpna1.na.infn.it

(antiferromagnet) Ising model (FF). The clusters so individuated allow us to generate MC algorithms for simulations of the FF and some results are presented in section 3. MC performances are explained examining cluster geometrical characteristics. Along these lines it is then possible to trace a panorama of possible successes and difficulties in applications to other more challenging systems.

## 1. Clusters and Ising spin systems

A well known example where clusters are introduced to study the properties of a system is the Ising ferromagnetic model (or more generally the unfrustrated Potts models). Kasteleyn and Fortuin (KF) [3], and later on Coniglio and Klein (CK) [4], have shown that it is possible to define clusters of spin in this way: if two spins satisfy their mutual interaction (i.e.  $S_i S_j = 1$ ) then you must put a bond between them ('freeze' the interaction) with probability  $p_{KF} = 1 - e^{-2\beta J}$  ( $J$  and  $\beta$  are, respectively, the spin pair interaction strength and the inverse temperature  $1/k_B T$ ), or else do not put any bond ('delete' the interaction). Then, after examining every couple of interacting spins, clusters are the maximal sets of spins linked by this kind of bond. Such clusters are characterized by a very important property:

$$\langle S_i S_j \rangle = \langle \gamma_{ij} \rangle \quad (1)$$

where  $\gamma_{ij}$  is one if sites  $i$  and  $j$  belong to the same cluster, and zero otherwise, and by definition  $\langle \gamma_{ij} \rangle$  is the connectivity function, i.e. the probability of the two sites  $i$  and  $j$  belonging to the same cluster. The above reported equation, which states the coincidence of spin thermodynamical correlation and connectivity of sites in the clusters, implies that the thermodynamical transition and percolative transitions belong to the same universality class and that their critical temperatures are equal,  $T_c = T_p$ .

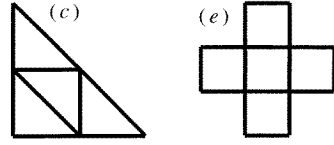
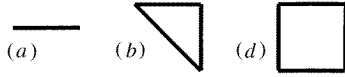
An important property of such clusters, very important for Monte Carlo cluster dynamics, is that they are absolutely not interacting [7]. So it is possible to implement easily an algorithm for a cluster MC dynamic as done in the cited pioneering work by Swendsen and Wang [6]. Such cluster algorithms, being based on clusters which exactly express the correlation between spins of the system, also allow coherent MC non-local updating at criticality, and so prevent critical slowing down.

It is easy to extend the above definition of clusters to frustrated and disordered Ising systems, described by a general Hamiltonian

$$H = - \sum_{\langle i,j \rangle} (J \epsilon_{ij} S_i S_j - J_0) \quad (2)$$

where  $\epsilon_{ij} = \pm 1$  is the interaction sign (chosen according to a given probability distribution),  $J \geq 0$  is the coupling modulus and  $J_0$  is a constant opportunely fixing the ground-state energy. Also in this case it is possible to define clusters as above, but whenever frustration is present, relation (1) is no longer valid and so thermodynamical and percolative transitions do not coincide [11]. To overcome such a problem you must be able to generate a wider class of possible clusters, and a natural step in this direction is to make less local moves for cluster building, i.e. to consider larger portions of the interaction lattice, as suggested by Kandel *et al* [10].

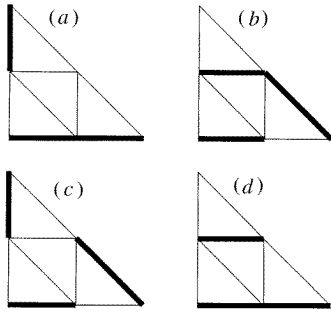
The procedure for cluster definition presented above in the form proposed by CK, can be repeated for every Hamiltonian that can be decomposed into a sum of basic units [10, 12] as  $H\{S_i\} = \sum_l H_l\{S_i\}$ , where the basic units  $H_l$  are elements of a partition of the whole interactions lattice, as a single pair of interacting spins as before, or plaquettes of nearest-neighbours spin, and so on (see figure 1). For each  $H_l$  we have to consider all the possible



**Figure 1.** Examples of possible units for partitions of a 2D triangular lattice (a), (b), (c), and a 2D square lattice (a), (d), (e). Each of them may be the starting point to map the corresponding spin system into a generalized percolation model (see the text). The KF approach is based on a lattice partition made only of single bonds as in (a).



**Figure 2.** The sets of ‘fundamental graphs’ of bonds for a frustrated triangular unit are (a) and (b) (see figure 1(b)). Only set (b) satisfies condition (8) and is adopted for the solution (10). Present bonds are marked by heavy lines and absent bonds by narrow lines.



**Figure 3.** The ‘fundamental graphs’ of a fully frustrated unit as in figure 1(c), compatible with conditions (8), may be obtained by rotations or reflection of those here depicted (the heavy lines are present bonds). Only the first three (with all possible rotation and reflections) have been adopted to write a solution given by equation (10) in which only graphs whose bonds are a subset of (a), (b) and (c) may have weights  $w_\alpha$  different from zero.

bond configurations in  $H_l$ , but, given the set of spins of  $H_l$ , a bond configuration is only allowed if in it all the pairs of interacting spin satisfy their mutual interaction. So, for example, the bond configuration with no bond present is always possible. Examples of bond configurations on lattice partition units are depicted in figures 2 and 3. To complete the scheme we have to introduce statistical weights  $w_\alpha$ , which are quantities to evaluate, for each bond configuration  $\alpha$  on  $H_l$ , and to obtain the equivalence of the original spin system with the new percolative model, to require that for each spin configuration  $\{S_i\}$  in  $H_l$  [12]:

$$\sum_{\alpha} w_{\alpha} \delta_{\alpha, \{S_i\}} = e^{-\beta H_l(\{S_i\})} \tag{3}$$

where the sum is extended to all bond configurations  $\alpha$ , and  $\delta_{\alpha, \{S_i\}}$  is 1 if the spin and bond configuration are compatible (i.e. if bonds are present only between a pair of spins satisfying their mutual interaction) and zero otherwise. It is important to note that equation (3) ensures that a Monte Carlo cluster random-flip dynamic based on such clusters verifies the *detailed balance principle* (DBP) [12] (in contrast, it is possible to prove that to impose DBP leads to (3) [10, 12]).

When frustration is present equation (1) must be substituted with the following [11, 12]:

$$\langle S_i S_j \rangle = \langle \gamma_{ij}^{\parallel} \rangle - \langle \gamma_{ij}^{\#} \rangle \tag{4}$$

where  $\gamma_{ij}^{\parallel}$  ( $\gamma_{ij}^{\#}$ ) is 1 if the spins  $i$  and  $j$  belong to the same cluster and are parallel (antiparallel), otherwise it is 0. Note that (4) generally implies  $|\langle S_i S_j \rangle| \leq \langle \gamma_{ij} \rangle = \langle \gamma_{ij}^{\parallel} \rangle + \langle \gamma_{ij}^{\#} \rangle$ .

The spin system may thus be mapped into a vast set of generalized percolation models [12, 16]. Equation (4) states that the clusters of these models generally do not resemble the correlation patterns in the system, but are just interfering fluctuations [11]. Equation (4) implies, moreover, that the critical thermodynamical temperature is always lower than or equal to the percolative one ( $T_c \leq T_p$ ) and so thermodynamical and percolative critical behaviour, for all the many solutions of equation (3), generally do not coincide.

However, it has been suggested elsewhere [12] that it is possible to exploit the redundancy of solutions of equation (3) to select those corresponding to cluster definitions which might give rise to efficient MC cluster dynamics. It was noted that a crucial point to this aim is to try to make the correlation and connectivity as equal as possible (and this corresponds to making  $T_p$  as near as possible to  $T_c$ ), in analogy to the Ising ferromagnet where percolative critical phenomena of KF or CK clusters coincide with the thermodynamical one (see equation (1)) and such clusters give rise to the efficient Swendsen and Wang MC dynamic.

Because  $|\langle S_i S_j \rangle| \leq \langle \gamma_{ij} \rangle$ , we must then try to select solutions of (3) in order to make connectivity as small as possible:

$$\langle \gamma_{ij} \rangle \rightarrow \text{minimum} \quad (5)$$

a condition which corresponds, roughly speaking, to shrinking clusters as much as possible, and is manifested by the indication of a  $T_p$  nearer and nearer to  $T_c$ . A direct search of the absolute minimum of equation (5), given the mapping relations (3), may be an extremely difficult task, but a simple consequent request in this direction is to try to impose that correlation and connectivity are equal at least on each single unit  $H_l$  of the partition of the lattice (KF or CK clusters verify this condition at least on any single spin pair interaction). The results of this choice should be better as the partition elements get larger (in the ideal case where the partition has just one element which coincides with the whole lattice, one should have the optimal situation  $|\langle S_i S_j \rangle| = \langle \gamma_{ij} \rangle$  as in an Ising ferromagnet). This requirement, expressed mathematically, leads to the following conditions to be imposed consistently with equation (3):

$$\langle \gamma_{ij} \rangle_l \rightarrow \text{minimum} \quad (6)$$

for each  $i$  and  $j$  on the  $l$ th block (the restriction of (5) to single partition units). Here

$$\langle \dots \rangle_l = \frac{\sum_{\alpha, \{S_i\}} \dots w_{\alpha} \delta_{\alpha, \{S_i\}}}{\sum_{\{S_i\}} e^{-\beta \mathcal{H}_l \{S_i\}}} \quad (7)$$

is the mean executed on the degree of freedom of just the  $l$ th block.

In [12] the following condition was introduced:

$$|\langle S_i S_j \rangle_l| = \langle \gamma_{ij} \rangle_l. \quad (8)$$

This would correspond to taking the ideal possible minimum in equation (6). However, there are some cases in which such an ideal minimum is not reachable and equation (8) leads to absurd results. These cases are often related to the specific choice of the lattice partition on which to impose equation (8), but a simple example is a partition of the square FF made of five plaquettes displaced on a cross (see figure 1(e)). In such an example it is possible to observe that condition (8) cannot be satisfied at  $T = 0$  and in the low temperature region.

So, even if equation (6) and (8) are in principle totally equivalent, in the sense that they should individuate the same subsets of solutions of equation (3), it is generally necessary

to adopt equation (6). However, in what follows, we will not meet such situations and conditions (6) and (8) will be equivalent.

The method for cluster definition based on the mapping equations (3) and conditions (8), introduced above, has proved successful [10,12] in the case of the 2D square fully frustrated lattice [17]. It was proved that cluster building from equation (3) for a lattice partition made of simple four-spin checkerboard plaquettes (see figure 1(d), imposing equation (8) (which at this level are totally equivalent to (6)), is enough to ensure that the thus generated percolation model has clusters with a percolation temperature  $T_p$  and critical percolative exponents numerically indistinguishable from  $T_c$  and the corresponding usual thermodynamical exponents (the geometric properties of a FF square lattice may have played a simplifying role [14]). The excellent performance of MC dynamics based on such clusters was ascribed to this property [10, 12, 14, 19].

As usual when disorder is added to frustration problems get harder. In the case of the 2D square  $\pm J$  Ising spin glass (SG) with  $T_c = 0$ , it was shown that under analogous conditions a good enhancement was possible but, as expected, the problem was not solved. Clusters built as in the SW algorithm have  $T_p = 1.8$  [20], while with this new technique used for a four spin plaquettes partition  $T_p = 1.2$ , allowing a great improvement in MC simulation at low temperature [12] if not also at criticality.

The rule to map the spin model in a percolation whose  $T_p$  is as near as possible to  $T_c$  then proves successful for simple frustrated systems but the problem is only partially solved in more difficult cases. In these situations it seems important to be able to take into account non-local effects linked to disorder and frustration. Relying on the crucial role of conditions (6) the natural further step to reach a wider equivalence of connectivity and correlation is to try to define clusters focusing the attention on larger lattice partition units (see figure 1) on which to impose the quoted conditions. The technical problem consists then in the increasing difficulty of proving the existence of positive solutions of the linear system of equation (3) and (6) if larger and larger lattice partition units are used.

In the next section a procedure for facing such a problem is described and example solutions are given in the case of a 2D triangular FF. Such solutions allow us to develop an efficient MC cluster dynamic in the FF (the SW dynamic is completely unsuccessful) whose performances are described in terms of the properties of the corresponding percolation model. The technique outlined below may be applied straightforwardly to other more complex spin systems and specifically to SG.

## 2. Explicit cluster definitions in the FF

The system of equations (3) grows exponentially with the size of the ‘basic unit’ of the lattice partition, but it always has solutions in the form of a factorized product of solutions of its subsections. This implies that KF weights for the cluster definition are always possible in a factorized form. For frustrated spin systems, however, the request to satisfy conditions (6) generally leads to this kind of solution being discarded.

The problem is solving, with positive  $w_\alpha$ , the coupled system of mapping equations (3) and conditions (8) or (6), may of course be greatly simplified exploiting the eventual rotational and reflection symmetries of the basic unit to choose the weights  $w_\alpha$  for the allowed configurations of bonds (for some more tricks to deal with the  $\langle \gamma_{ij} \rangle_l$  see [12]). But a crucial observation to find solutions of such a system is to note that the form itself of (3) implies, at  $T = 0$ , that only a few bond graphs  $\alpha$  have weight  $w_\alpha(T = 0)$  different from zero, i.e. those appearing exclusively in the equations of (3) which correspond to ground-state spin configurations on the basic partition units. This drives from the fact that the

right-hand side of equation (3) at  $T = 0$  is zero unless one evaluates it on a ground state. To simplify notations let us call such bond graphs ‘fundamental graphs’ (see the examples in figures 2 and 3).

Moreover, many ‘fundamental graphs’ are discarded (i.e. assigned a zero weight) under conditions (6) or (8) (see figure 2). As a matter of fact, such a  $T = 0$  analysis is an easy pre-test to understand if it is possible to impose all equations (8), unconditionally or if it is necessary to adopt the less restrictive conditions (6) to avoid finding it absurd discarding too many graphs.

In the case of a 2D triangular isotropic FF lattice [17] (i.e. a 2D triangular isotropic antiferromagnet) if the partition is made of three spin ‘single plaquette’ as basic units (see figure 1(b)), these prescriptions lead straightforwardly to the following unique solution of (3) and (8) in the range  $T \in [0, \infty]$  (see figure 2):

$$\begin{aligned} w_0 &= e^{-4\beta J} \\ w_1 &= (1 - e^{-4\beta J})/2 \\ w_2 &= w_3 = 0 \end{aligned} \quad (9)$$

where  $w_\alpha$  ( $\alpha = 0, 1, 2, 3$ ) is the weight of configurations with a number of bonds  $\alpha$  (this solution was found previously in a different way in [19]).

If the partition of the 2D triangular FF lattice is made of larger basic units consisting of ‘three plaquettes’ of six spin, as in figure 1(c), it is possible to find many solutions of equations (3) and (8), however, at low temperature they differ at most for terms of the order of  $e^{-4\beta J}$ . Following the previous reasoning we at first individuate the ‘fundamental graphs’ compatible with conditions (8) (see figure 3). Then to easily obtain solutions  $\{w_\alpha\}$ , we impose  $w_\alpha = 0$  for each bond configuration  $\alpha$  which is not a subgraph of these ‘fundamental graphs’ satisfying (8). Consequently, all the allowed bond configurations by definition satisfy (8) (i.e. equation (6)) for all values of  $T$ , because in our case the  $\langle S_i S_j \rangle_l$  do not change sign with  $T$ .

According to these simple rules, it is possible to obtain many solutions and here I present a simplified version based on just three of the four kinds of ‘fundamental graphs’ allowed for a ‘three plaquettes’ unit on a FF (see figure 3) so to have to deal with the lowest number of graphs (the excluded ‘fundamental graph’, depicted in figure 3(d), has zero weight at  $T = 0$ ). To further distinguish different bond graphs I used the above quoted symmetry arguments, and so characterized them by two indices  $(h, k)$  of which the first indicates the total number of bonds of the graph and the second the ‘fundamental graphs’ of which it is a subgraph. In more complex cases better discrimination may be useful, but the main line is similar to the simple one outlined here to easily explain the procedure.

The following solution is valid in the range (in units  $J/K_B$ )  $0 \leq T \leq 31.958$  (we are interested in the low temperature region), and was selected among the others for the very low number of different graphs it includes (it has just 48 different graphs, while the FF solution for the same unfrustrated unit has 512 graphs, see figure 3):

$$\begin{aligned} w_{0,7} &= x^3 \\ w_{1,7} &= x^2(1-x)/2 \\ w_{1,2} &= 11x^2(1-x)/20 \\ w_{2,1} &= w_{2,7} = x(1-x)^2/4 \\ w_{2,2} &= x(15-32x+17x^2)/40 \\ w_{3,4} &= w_{3,1} = (1-x)^3/8 \\ w_{3,2} &= (15-55x+69x^2-29x^3)/40 \end{aligned} \quad (10)$$

with all other  $w_{h,k}$  equal to zero ( $h = 0, 1, \dots, 9$   $k = 1, 2, \dots, 7$ ) and  $x = e^{-4\beta J}$ . Specifically,  $k = \sum_i b_i 2^{i-1}$ , where  $i = 1, 2, 3$  is the ordering number of the exploited fundamental graphs (respectively depicted in figures 3(a)–(c) and  $b_i$  is one if the bond configuration is a subgraph of the  $i$ th fundamental graph and zero otherwise (see figure 3);  $h$  is, as just stated, the total number of bonds of the configuration (different graphs with the same  $h$  and  $k$  are considered equivalent and have the same statistical weight). So, for example,  $w_{1,7}$  is the weight of the graphs which have one bond and are a subgraph of ‘fundamental graphs’ number 1, 2 and 3. Note that solution (10) is not just a trivial product of solution (10), and that the net effect of conditions (6) or (8) is to make clusters as filiform as possible.

According to the given prescription, the problem of discriminating between the exponentially large number of possible graphs on the basic units is primarily reduced to the determination of special classes of ‘fundamental graphs’ as indicated by the formal properties of equation (3), graphs strictly related to the structure itself of spin ground states on the basic units.

### 3. Monte Carlo results

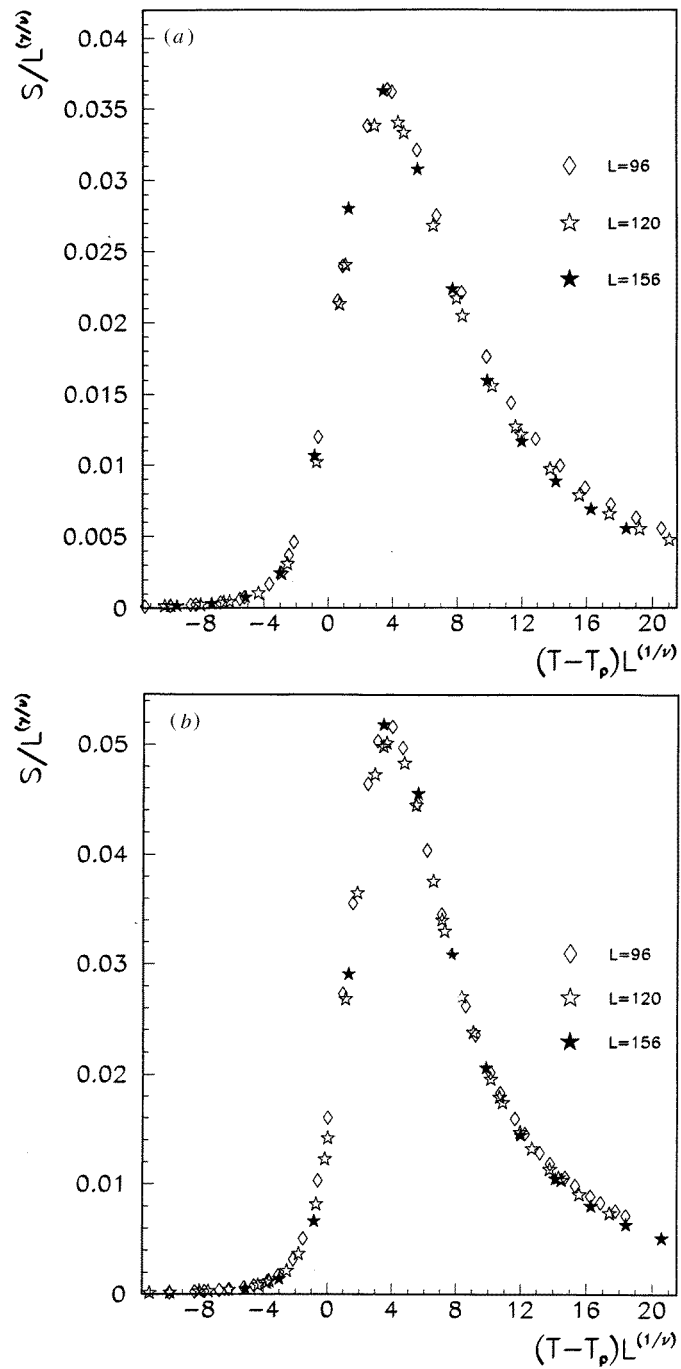
The results of the previous section may be important in understanding if the criterion to exploit larger and larger units in the partition of the spin lattice to build clusters, which satisfy conditions (6) allows us to define in successive approximation clusters percolation critical properties as near as possible to the spin critical one. We are also interested to verify if such a criterion is well grounded to individuate efficient MC cluster dynamics and, moreover, if it has a reasonably fast convergence. A clear marker of its success in individuating ‘good’ clusters is its efficiency in pushing  $T_p$  towards  $T_c$ .

Examining the properties of the cluster defined in the previous section, we can derive some information in these directions in the case of the two-dimensional triangular FF and thus formulate a possible panorama for more complex spin systems. Using MC simulations it is possible to easily estimate, for the clusters defined above, the percolation temperature  $T_p$  where the mean cluster size  $S$  diverges.  $S$  is defined as  $S = \sum'_s n_s s^2$ , where  $n_s$  is the mean number of clusters of size  $s$ , and  $\sum'_s$  is the sum over all clusters of finite size [15]. Our MC simulations were based on both standard Metropolis and the presented cluster algorithms. The lattice sizes  $L$  considered were in the range  $48 \leq L \leq 156$  (in some cases  $48 \leq L \leq 240$ ). The number of MC lattice updates per run was, depending on  $L$  and  $T$ , of about  $10^5$  after  $10^4$  were discarded to equilibrate the system. With a finite-size scaling analysis [18] I found the following results:

$$T_{p_0} = 2.5 \pm 0.1 \quad T_{p_1} = 1.23 \pm 0.05 \quad T_{p_2} = 0.93 \pm 0.05 \quad (11)$$

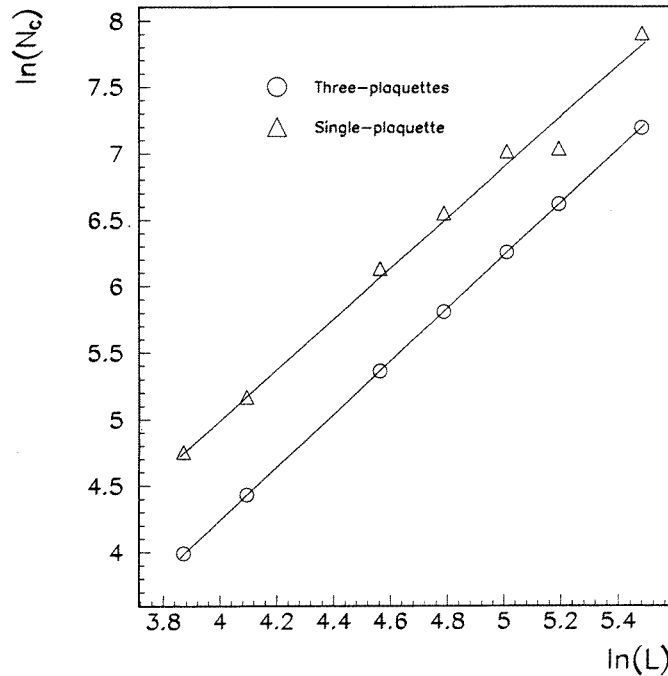
where  $T_{p_0}$  is the percolation temperature for KF (i.e. CK or SW) pioneering clusters (figure 1(a)),  $T_{p_1}$  for clusters built adopting as a basic unit a ‘single plaquette’ (figure 1(b)) and weights given by (10), and  $T_{p_2}$  for clusters based on the larger partition unit of ‘three plaquettes’ (figure 1(c)) characterized by equations (10) (temperatures are measured in absolute units  $J/k_B$ ). In all these cases, as expected  $T_p > T_c = 0$ , the critical percolative exponents of the cluster mean square radius  $\nu$  and mean cluster size  $\gamma$  are in the 2D random bond percolation universality class  $\nu = \frac{4}{3}$  and  $\gamma = \frac{43}{18}$ , and equal to  $\nu = 1.33 \pm 0.03$  and  $\gamma/\nu = 1.90 \pm 0.05$  for the ‘single plaquette’ case and  $\nu = 1.33 \pm 0.03$   $\gamma/\nu = 1.85 \pm 0.05$  for the ‘three plaquettes’ one. This is illustrated in figure 4 where the finite-size scaling analysis for the mean cluster size  $S$  of ‘single’ and ‘three plaquettes’ based clusters is reported. Such a result means physically that there are no thermodynamical effects underlying the percolative





**Figure 4.** Finite-size scaling of the mean cluster size  $S$  for (a) 'single' and (b) 'three plaquettes' built clusters (i.e. clusters from equations (10) and (10), respectively). In case (a)  $T_p = 1.23 \pm 0.05$  while in case (b)  $T_p = 0.93 \pm 0.05$ . Percolative exponents are, in the range of errors, equal to those of random percolation.

transition. It is important to stress that the lowering of  $T_p$  corresponds to an increase in



**Figure 5.** The logarithm of the mean number of clusters  $N_c$  in the system at  $T = T_c = 0$  as a function of the logarithm of the linear system size  $L$ , for 'single' (triangle) and 'three plaquettes' (circle) built clusters. In both cases  $N_c$  grows quadratically with  $L$  (see the text). Straight lines are best-fit linear interpolations.

the performance of MC cluster dynamics (see below) based on the presented definitions of clusters equations ((10) and (10)), also if the slow convergence of  $T_p$  toward  $T_c = 0$  clearly indicates the kind of difficulties one must expect in the case of more complex systems as disordered and frustrated ones.

Another important phenomenon is to be noted: while KF clusters below  $T \sim 1$  froze the whole lattice in a single huge cluster, in the case of the 'single plaquette' and 'three plaquettes' based clusters, also at  $T = 0$ , there are many independent clusters. At  $T = 0$  the mean number of clusters  $N_c$  scales as (see figure 5):

$$N_c = AL^\mu \quad (12)$$

with  $\mu \sim 2$ , and specifically  $\mu = 1.9 \pm 0.1$  and  $A = 0.07 \pm 0.02$  in the 'single plaquette' case and  $\mu = 1.99 \pm 0.07$  and  $A = 0.025 \pm 0.007$  in the 'three plaquettes' one. This behaviour is consistent with the observation that the largest cluster does not cover the whole lattice even at  $T = 0$ . It is possible to see that at  $T = 0$  the largest cluster in the system, which is the only one to percolate, follows a scaling law like  $S_{max} = BL^2$  where  $S_{max}$  is the mean number of spins which belong to it and  $L$  the lattice size. MC results give  $B = 0.924 \pm 0.002$  for 'single plaquette' and  $B = 0.944 \pm 0.001$  for 'three plaquette' clusters (for KF it is  $B = 1$ ).

For the lattice sizes  $L \leq 240$  which I explored, MC data from preliminary runs of light statistic ( $3 \times 10^5$  MCS) show at  $T = 0$  fractal behaviour for mean numbers of spins  $S_{II}$  in the second largest cluster of the system,  $S_{II} = CL^{D_{II}}$ , with  $D_{II} \sim 0.6$  for both 'single' and 'three plaquettes' case.

The above presented phenomenon, and specifically the existence of a huge number of clusters also at  $T = T_c = 0$ , has an important consequence on MC cluster dynamic performances. While SW cluster dynamic results are totally inefficient, freezing the lattice in a single cluster, preliminary runs show that MC dynamics based on clusters from equations (10) and (10) are also active at  $T = 0$ . Their decorrelation times are of the order (smaller for temperatures higher than  $T^* \sim 0.4$ ) of those of a standard Metropolis single spin-flip dynamic [19] (autocorrelation times for the square magnetization are extremely low even at  $T = 0$ , a few MC step per spin).

The fact that dynamical times of ‘single’ and ‘three plaquettes’ based MC dynamics are comparable to Metropolis, is to be expected: their clusters do not express the correlations in the systems because of the finite gap between  $T_p$  and  $T_c$ , but they flip many clusters ( $N_c \sim L^2$ ) also at  $T_c = 0$  and so their moves are substantially equivalent to a normal Metropolis.

The slow convergence of  $T_p$  towards  $T_c$  is then (at least partially) compensated by the existence of a great number of clusters also at  $T_c$ . This new phenomenon originated by the geometry of the new clusters then has an important consequence on the MC cluster dynamics’ performance. The favourable properties of the presented clusters are strictly related to the fact that they obey conditions (6) via (8): in fact, solutions of (3) chosen according to merely ‘reasonable’ arguments, have proved completely wrong [19], having properties substantially equal to those of the simple KF (i.e. CK or SW) clusters.

#### 4. Discussion and conclusions

This paper has been focused on the problem of mapping spin systems into percolation models to individuate clusters with suitable properties to give a percolation description of the spin-critical phenomenon, and to test the applicability of some new general criterion to build general MC efficient cluster dynamics [12]. This mapping was realized through the generalization of the Kasteleyn and Fortuin formalism given by equation (3). The many solutions of such a mapping were selected according to condition (6), whose crucial role was stressed. This condition is based on the recent idea that to obtain clusters suitable for efficient MC dynamics it is highly useful to select them in order to make their percolation connectivity function as similar as possible to the spin correlation function [12].

A procedure to solve the system of mapping equation (3) and conditions (8) (if conditions (8) can be satisfied, they are equivalent to (6)) has also been presented and explicit solutions in the case of 2D triangular FF given in (10) and (10).

This quoted scheme for suitable cluster individuation in Ising systems, has, in fact, a wide generality, and also the technical procedure to get explicit definitions, presented for the FF, results from an easy implementation in general frustrated Ising systems. An interesting and straightforward application of it would be, for instance, to 2D triangular SG where the complication with respect to the case dealt with here consists in the mere necessity of considering the various kinds of ‘basic units’ of the lattice partition and not just the fully frustrated one. An application of these methods has also been exploited in frustrated XY models [21].

From the explicit solutions given for the FF, new clusters definitions were introduced in such system, whose percolation point  $T_p$  was, in fact, systematically lowered towards the critical one  $T_c$ , as expressed in (11). Moreover, in contrast to the SW cluster dynamic, MC cluster algorithms based on such solutions, even if not optimal because of the finite gap  $T_p - T_c$ , for their specific geometrical properties do not freeze the system even at criticality and, in the FF, result comparable to Metropolis single spin flip. Being  $T_p > T_c$ , this result

is not surprising as discussed above, and the evident improvement obtained with respect to the SW dynamic and the success in narrowing the gap  $T_p - T_c$  should encourage the research of faster and faster cluster algorithms in the low  $T$  region of frustrated systems. It would be interesting to make a more detailed study of time properties of such cluster dynamics in these systems where the Metropolis critical slowing down exponent  $z$  is very high.

So, even if the slow convergence of  $T_p$  towards  $T_c$  found in the FF signals the difficulties to be faced in the applications of such methods to more complex cases, at the same time, the possibility of substantially reducing  $T_p$  may give rise to very efficient MC explorations of the low temperature region in these systems, even if not exactly at  $T_c$ .

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