PHYSICA A

Percolation and cluster formalism in continuous spin systems

Mario Nicodemi *

Dipartimento di Scienze Fisiche, Università di Napoli, Mostra d'Oltremare Pad.19, I-80125 Napoli, Italy
Sezione INFM and INFN di Napoli, Italy

Abstract

The generalization of Kasteleyn and Fortuin clusters formalism is introduced in XY (or more generally $O(n)$) models. The clusters' geometrical structure may be linked to spin physical properties as correlation functions. To investigate percolative characteristics, the new cluster definition is analytically explored in one dimension and with Monte Carlo simulations in 2D and 3D frustrated and unfrustrated n-clock models.

1. Introduction

The idea to describe long range correlations and coherency in spin systems from a geometrical point of view dates back to thirty years. In the late 1960s this project was accomplished for Ising models by Kasteleyn and Fortuin (KF), who developed a method to give intrinsic definitions of clusters of spins which might describe with their percolation characteristics the structure of correlations patterns. Cluster formalism and percolation tools [1,2], have proven extremely useful in the understanding of critical phenomena of Ising models [3,4]. Among the many results, very interesting is the discovery of the possibility to describe spin correlations through percolative connectivity functions and the consequent link between thermodynamic critical behaviors and cluster fractal structures (see [5]). The individualization of "physical" clusters of spin introduced within this approach, has been also successfully exploited by Swendsen and Wang (SW) [6,7] to develop fast Monte Carlo (MC) dynamics, for unfrustrated Ising models, based on cluster update and later on to drastically improve simulations in frustrated systems too [8,9].

Nevertheless, the discussions about the extension of cluster formalism and percolation concepts to continuous spin systems as XY or $O(n)$ models is still open, and the

---

* E-mail: nicodemim@axpna1.na.infn.it.

equivalent of KF cluster in such systems is not known. Wolff [7] has proposed a cluster definition in XY models based on a smart application of KF rule to spin projections along random directions. The clusters so introduced have proven to have a percolative critical temperature exactly equal to the thermodynamic one in unfrustrated XY models, also if their ultimate connections with spin properties is not understood [11]. One of the successes of KF approach consists in the clarification of the links between the clusters and the physics of the spins.

In this paper we try to address a possible generalization to XY and $O(n)$ models of KF approach to Ising-like systems. This extension leads to new cluster definitions. In the spirit of the works of Kasteleyn–Fortuin and Coniglio–Klein (CK) we try to focus the relations between clusters and spins, disregarding, at the moment, applications to efficient MC algorithms. Specifically, we try to introduce concepts and tools to manipulate the structure of such clusters in this larger context, as done by KF and CK in Ising-like systems. In ferromagnetic models, the new clusters generally individualize regions of statistically coherent spins, i.e. almost parallel spins, and describe the physics of such aggregates. For the sake of clarity, before passing to such a generalization (presented in Sections 3 and 4), in Section 2 a fast outlook at the original KF approach to Ising systems is given, to define notations and concepts used in what follows. Later, the properties of these new clusters are analytically studied in one dimension and via MC simulations in n-clock models in 2D and 3D, where the thermodynamic transitions have different properties.

2. Cluster formalism for Ising spin Hamiltonians

Let us consider an Ising system of spins $S_i = \pm 1$ with the Hamiltonian:

$$\beta \mathscr{H}(\{S_i\}) = -\sum_{\langle i,j \rangle} (J_{ij} S_i S_j - |J_{ij}|), \tag{1}$$

where $\{S_i\}$ is the spin configuration, the sum is over all interacting spin pairs and, as usual, $\beta = 1/k_B T$. The constants in the Hamiltonian have been chosen for future convenience and for simplicity we can consider $J_{ij} = J > 0 \ \forall i,j$, i.e. we take an Ising isotropic ferromagnet.

The cluster formalism to describe "droplets" of Ising spin [3] was originally developed by Kasteleyn and Fortuin [1], and later on in a different approach by Coniglio and Klein [2]. It is based on the mapping of the original model described by Hamiltonian (1) into a new model in which spin couplings have infinite or zero strength. The mapping consists in stochastically changing the interactions J_{ij} between spin pairs to new values J'_{ij} (to define clusters we are interested in the limit $|J'_{ij}| \to \infty$ or $J'_{ij} \to 0$), in such a way that the two models, with new and old interactions, are statistically equivalent.

Towards this aim, following KF, let us consider then each pair of interacting spins S_i and S_j, and suppose $J'_{ij} \in \{0, J', -J'\}$ with $J' > 0$. If the change of J_{ij} to a new

interaction $J'_{ij} = J'$ occurs with a weight p_0, to a $J'_{ij} = -J'$ with p_π and to $J'_{ij} = 0$ with q, then the sum of statistical weights of a spin configuration $\{S_i, S_j\}$ in the new possible models is [1,2]

$$W(S_i, S_j) = q + p_0 e^{J'(S_i S_j - 1)} + p_\pi e^{-J'(S_i S_j + 1)} . \tag{2}$$

It is to be noticed that we are slightly modifying the original KF–CK approach in which p_π was a priori set to zero. To impose the statistical equivalence of the original and mapping models we must then require that a given spin configuration has the same weight:

$$\exp(-\beta \mathcal{H}(\{S_i\})) = \prod_{\langle i,j \rangle} W(S_i, S_j) . \tag{3}$$

So for each pair of interacting spins we must require:

$$e^{J(S_i S_j - 1)} = q + p_0 e^{J'(S_i S_j - 1)} + p_\pi e^{-J'(S_i S_j + 1)}, \tag{4}$$

where the p_0, p_π and q are unknown temperature functions.

To introduce the definition of clusters of spins we must consider the limit $J' \to \infty$. Two spins S_i and S_j connected in the new model by an infinite interaction must have then a definite reciprocal direction (i.e. parallel if $J'_{ij} = +J'$ and antiparallel if $J'_{ij} = -J'$) to have a nonzero weight, otherwise, if disconnected, they are completely independent. Thus in the new model the *clusters* are naturally defined as the maximal sets of spins connected by ∞ interactions (called *bonds*). The *deletion* ($J'_{ij} = 0$) or the *freezing* ($|J'_{ij}| = \infty$) of the original interactions leads to the contraction of the spin lattice in independent fundamental units: the clusters. In the limit $J' \to \infty$, Eq. (4) becomes:

$$e^{J(S_i S_j - 1)} = q + p_0 \delta_{S_i, S_j} + p_\pi \delta_{S_i, -S_j} . \tag{5}$$

This is a linear system of two equations with three unknowns q, p_0 and p_π, and so it is possible to introduce physical constraints to select some definite solution [9]. Towards this aim let us introduce the connectivity function γ_{ij}, which is one if spin S_i and S_j belong to the same cluster and zero otherwise. It is possible to show that connectivity is always greater or equal to spin correlation [9,12]:

$$\langle S_i S_j \rangle = \langle \gamma_{ij}^{\parallel} \rangle - \langle \gamma_{ij}^{\nparallel} \rangle \leqslant \langle \gamma_{ij}^{\parallel} \rangle + \langle \gamma_{ij}^{\nparallel} \rangle \equiv \langle \gamma_{ij} \rangle , \tag{6}$$

where $\gamma_{ij}^{\parallel}$ ($\gamma_{ij}^{\nparallel}$) is one if S_i and S_j belong to the same cluster and are parallel (antiparallel). A criterion which proved to be extremely important to select the definitions of interacting clusters (i.e. the relative value of q, p_0 and p_π) is to make connectivity as close as possible to correlation, i.e. to minimize connectivity as a function of q, p_0 and p_π [9,14]:

$$\langle \gamma_{ij} \rangle \to \text{minimum} . \tag{7}$$

This natural condition, which corresponds essentially to selecting clusters whose structure resembles the correlation patterns in the system, has given excellent results in

frustrated and unfrustrated Ising spin systems [9,14]. In the case of the simplest approximation in which we consider just a single couple of interacting spins S_i and S_j, the mean connectivity is $\langle \gamma_{ij} \rangle = (p_0 + p_\pi)/(1 + e^{-2J})$, and to impose condition (7), with constraints $0 \leqslant q, p_0, p_\pi$, naturally leads to $p_\pi = 0$ (or analogously $p_0 = 0$ if $J < 0$). In the present case, this result also may be simply obtained by directly imposing $\langle S_i S_j \rangle = \langle \gamma_{ij} \rangle$. The solution:

$$p_\pi = 0; \qquad p_0 = 1 - q = 1 - e^{-2J} \tag{8}$$

is the well known result of Kasteleyn–Fortuin [1] and Coniglio–Klein [2]. Within this context it is possible to show that the partition function of a Q-Potts model [4] may be written as ($Q = 2$ corresponds to Ising model) [1,2]:

$$Z_Q(J) = \sum_C q^{|A|} p_0^{|C|} Q^{N(C)} , \tag{9}$$

where $p_0 = 1 - e^{-QJ} = 1 - q$, $N(C)$ is the number of clusters in the configuration of bonds C (i.e. the set of ∞ interactions), $|C|$ (resp. $|A|$) is the total number of bonds in C (resp. of absent bonds or zero interactions), and $\sum_C$ is the sum over all bonds configurations. Eq. (9) gives the Ising partition function in terms of the partition function of a correlated-percolation model [13]. Moreover, with KF solution, for an Ising ferromagnet, Eq. (6) becomes:

$$\langle S_i S_j \rangle = \langle \gamma_{ij} \rangle . \tag{10}$$

3. Cluster formalism for XY spin Hamiltonians

Let us examine now the problem of cluster definitions in continuous spin systems. We consider an XY model, but the same arguments may be extended to $O(n)$ models. Specifically, we consider a system of planar spins, S_i, with pair Hamiltonian:

$$\beta H_{ij} = -(J_{ij} \cos(\theta_i - \theta_j) - |J_{ij}|) , \tag{11}$$

where θ_i is the phase of spin S_i, as before we take $\beta = 1/k_B T$ and for clarity $J_{ij} = J > 0$. The constant in the Hamiltonian has been chosen for convenience so that two ferromagnetically interacting spins have zero energy when they are parallel.

Following the idea proposed by KF, we map the original model described by Hamiltonian (11) into a new model in which the pair Hamiltonian between interacting spins is stochastically changed to new functional values H'_{ij}, in such a way that the two models are statistically equivalent. As above, to individuate clusters we are interested in the limit $H'_{ij} \to \infty$ or $H'_{ij} \to 0$. The main difference with the previous section consists in the fact that many choices for H' are necessary, but the arguments will be the same. Let us therefore define new pair Hamiltonians characterized by a new variable ϕ'_{ij}:

$$\beta H(S_i, S_j; \phi'_{ij}) \equiv -(J'_{ij} \cos(\theta_i - \theta_j - \phi'_{ij}) - |J'_{ij}|) + C(J'_{ij}) , \tag{12}$$

where the parameter is $\phi'_{ij} \in [0, 2\pi]$, $J'_{ij} = J' > 0$ and $C(J')$ is an adjustable regularization function in the limit $J' \to \infty$.

To impose the statistical equivalence of the original and the mapping models, we then require that spin configurations have the same weight in both of them, so if we define $p(\phi')$ as the statistical weight to map the pair Hamiltonian (11) into $H(S_i, S_j; \phi')$, and q the weight to map it into a zero energy interaction, then Eq. (4) becomes

$$e^{-\beta H_{ij}(S_i, S_j)} = q + \int_0^{2\pi} p(\phi') e^{-\beta H(S_i, S_j; \phi')} \, d\phi' \, . \tag{13}$$

As above, to define clusters we consider the limit $J' \to \infty$. Two spins S_i and S_j connected in the new model $H(S_i, S_j; \phi'_{ij})$ by an infinite interaction, must have a definite reciprocal direction (i.e. $\theta_i - \theta_j = \phi'_{ij}$) to have a nonzero weight; otherwise, if not connected, they are completely independent. Thus in the new model the *clusters* are naturally defined as the maximal sets of spins connected by ∞ interactions (*bonds*). In contrast to the Ising case we now have much more than just two kinds of bonds (between parallel spins p_0, or antiparallel spins, p_π). Following this method it is then possible to generalize the procedure of *deletion* ($J'_{ij} = 0$) and *freezing* ($J'_{ij} = \infty$) of the original interactions. Also in this case different clusters are independent (if q is a function of $\theta_i - \theta_j$ or if the infinite limit is not systematically taken, then one has interacting clusters). In the infinite limit $J' \to \infty$, Eq. (13) becomes

$$e^{-\beta H_{ij}(S_i, S_j)} = q + \int_0^{2\pi} p(\phi') \delta(\theta_i - \theta_j - \phi') \, d\phi' = q + p(\theta_i - \theta_j) \, , \tag{14}$$

where the function $C(J')$ has been absorbed to regularize the definition of the δ-function in the interval $[0, 2\pi]$ with argument defined modulus 2π. Eq. (14) is a linear functional equation in the unknown functions $p(\phi', J_{ij})$ and $q(J_{ij})$.

A solution of Eq. (14) is suggested by the reasonable limit behavior $p(\phi') \to 0$ if $J \to 0$, or alternatively by the condition of local minimal connectivity (see below):

$$q = e^{-2J}; \qquad p(\phi') = e^{J(\cos(\phi') - 1)} - q \, . \tag{15}$$

This solution reproduces in the Ising case the results by Kasteleyn and Fortuin given in Eq. (8).

The clusters are operatively individualized by the conditioned probabilities:

$$p(\phi' | \theta_i - \theta_j) = p(\phi') \delta(\theta_i - \theta_j - \phi') e^{\beta H(S_i, S_j)};$$
$$q(\theta_i - \theta_j) = q \cdot e^{\beta H(S_i, S_j)} \tag{16}$$

which may be interpreted as the conditioned probability to substitute the original interaction in the mapping model with a bond of the kind ϕ' or with a zero interaction, given the spin configuration $\{S_i, S_j\}$ (note that these probabilities are completely independent of the choice of the constants for the energy of the ground state). These

conditioned probabilities may be used to implement MC cluster algorithms because they contain the necessary information to build clusters from spin configurations and it may be proved that algorithms based on these probabilities satisfy detailed balance principle [8,9]. They are the generalization to *XY* of KF bond conditional probabilities in Ising systems.

Eq. (14) may also be considered directly as the starting point to define clusters of bond variables $\{\phi'_{ij}\}$, avoiding completely to introduce the procedures of Hamiltonian mapping and definitions (12). In this perspective Eq. (14) is just a way to introduce a statistical system of variables of spin and bonds ($\{\theta_i\}, \{\phi'_{ij}\}$) with the following peculiar properties [15]: the marginal distribution of the $\{\theta_i\}$ is exactly equal to the Boltzman weight $e^{-\beta H(\{\theta_i\})}$; the conditional distribution of $\{\phi'_{ij}\}$, given $\{\theta_i\}$, is exactly expressed by Eqs. (16); the conditional distribution of $\{\theta_i\}$, given $\{\phi'_{ij}\}$, corresponds to the above given definition of clusters, i.e. two interacting spin S_i and S_j belonging to the same cluster must have a definite reciprocal direction $\theta_i - \theta_j = \phi'_{ij}$; otherwise, if disconnected, they are completely independent. Note that only the sets $\{\phi'_{ij}\}$, such that given any two sites h and k the quantity $\Delta\theta = \sum_h^k \phi'_{ij}$ is independent of the "integration" path, are allowed.

4. Relations between thermodynamics and percolation

The previous section was devoted to introduce a simple generalization of Kasteleyn–Fortuin and Coniglio–Klein clusters in *XY* models. Now we face the problem of working out some main relations between percolative and thermodynamic quantities. Easy extensions may be given for general $O(n)$ models.

The partition function of the *XY* model, from Eq. (14), may be written as

$$Z \equiv \prod_i \int_0^{2\pi} d\theta_i\, e^{-\beta \sum_{\langle i,l\rangle} H(S_i, S_j)} = \sum_{\tilde{C}}^* q^{|A|} P(\tilde{C})(2\pi)^{N(\tilde{C})}\,, \tag{17}$$

where $|A|$ is the number of bonds absent on the fixed lattice configuration $\tilde{C}$, $N(\tilde{C})$ is the total number of clusters in $\tilde{C}$, and by definition $P(\tilde{C}) = \prod_{\langle ij\rangle \in \tilde{C}} p(\phi'_{ij})$. The sum, $\sum_{\tilde{C}}^*$, is intended over all possible bond configurations, $\tilde{C}$ (note that two bond configurations are distinguished by their geometry and by the kind of bonds $\{\phi'_{ij}\}$ they have), and specifically

$$\sum_{\tilde{C}}^* \equiv \sum_{\tilde{C}} \int \left(\prod_{\langle ij\rangle \in \tilde{C}} d\phi'_{ij} \right) \delta(\tilde{C}, \{\phi'_{ij}\}) \tag{18}$$

with $\prod_{\langle ij\rangle \in \tilde{C}}$ the product over all bonds present in the configuration $\tilde{C}$, $\{\phi'_{ij}\}$ the set of indexes of such bonds present and $\delta(\tilde{C}, \{\phi'_{ij}\})$ a function nonzero only if the configuration $\tilde{C}$ and the set $\{\phi'_{ij}\}$ are compatible (i.e. if the sum of ϕ'_{ij} between whatever fixed extrema h and k along a chain of present bonds, is independent of

the path, i.e. clusters are well defined because such a quantity is exactly the phase difference between S_h and S_k).

The percolative quantity to be compared to the thermodynamic two point correlation function is the pair connectivity $c(i,j)$, defined as

$$c(i,j) = \int_0^{2\pi} c(i,j,\phi)\,d\phi \,, \tag{19}$$

where $c(i,j,\phi) = \langle \gamma_{ij}(\phi) \rangle$ and $\gamma_{ij}(\phi) = \gamma_{ij} \cdot \delta(\theta_i - \theta_j - \phi)$ which is zero if the spins S_i and S_j do not belong to the same cluster or have a phase difference $\theta_i - \theta_j \neq \phi$. $c(i,j,\phi)$ is therefore the probability of spin i and j to belong to the same cluster with a phase difference ϕ.

It is possible to show that the pair correlation function $g(i,j) = \langle S_i \cdot S_j \rangle$ is given by

$$g(i,j) = \int_0^{2\pi} \cos(\phi) c(i,j,\phi)\,d\phi \,. \tag{20}$$

Eqs. (19) and (20) imply $g(i,j) \leqslant c(i,j)$, analogously to Ising systems where Eq. (6) holds. A consequence of this proven inequality is that $T_c \leqslant T_p$, where T_c and T_p are defined as the temperatures where the magnetic susceptivity χ and the mean cluster size $S = \sum_s' n_s s^2$ [13] (n_s is the number of clusters of size s and $\sum_s'$ is the sum over just finite clusters) become singular, respectively. These relations naturally suggest, in analogy with the Ising spin case, the criterion of minimal connectivity to select cluster definitions, i.e. to impose the condition:

$$c(i,j) \rightarrow \text{minimum} \,, \tag{21}$$

where $c(i,j)$ has to be minimized respect to $p(\phi)$. As anticipated above, imposing Eq. (21) just for each pair of interacting spins S_i and S_j, directly leads to select the solution given in Eq. (15) for Eq. (14). It is to be noticed that this solution is however just the simplest extensions of the KF result. In fact more general solutions must be found as shown below, but the general tools introduced to link percolative and spin properties, allows to exploit, for XY models, the many techniques to individualize and manipulate clusters known in the literature for Ising systems (see [1,2,9,14]). In what follows we will restrict, however, to consider the simple solution given in Eq. (15).

The relations reported above indicate that thermodynamic spin quantities may be generally expressed in terms of cluster properties. For example it is possible to link the mean energy E with geometrical quantities. In the case of an isotropic ferromagnetic XY model it gives

$$E/N = -\langle \gamma_{01} \partial_\beta \ln(p(\phi'_{01})/q) \rangle + \partial_\beta \ln(q) \,, \tag{22}$$

where 0 and 1 are two of the N interacting pairs of spin in the system. As Eq. (17) is the natural generalization of Eq. (9), so is Eq. (22) the extension of the corresponding energy-bond relation in Ising systems [9,16].

5. Clusters in a one-dimensional XY model

To understand the properties of the above defined clusters it may be interesting to analyze the question in some details. In a one-dimensional XY model of nearest neighbor interacting spins [17], the geometry of the above defined clusters corresponds to chains of bonds, and the problem is extremely simplified. So it is possible to prove that, adopting solution (15), the partition function, Eq. (17), in the case of an isotropic XY ferromagnetic chain, is

$$Z_{1D}(J) = \sum_{C} q^{|A|} P^{|C|} (2\pi)^{N(C)} , \qquad (23)$$

where $\sum_{C}$ is just the sum over all graphs of bonds on the chain, $P = 2\pi e^{-J}(I_0(J) - e^{-J})$ ($I_n(x)$ is the imaginary argument Bessel function of order n). From Eq. (23) it is possible to see that the partition function of an XY chain may be written as that of a Q-Potts linear model, Z_Q (see Eq. (9)), times a simple factor. Specifically,

$$Z_{1D}(J) = K \cdot Z_Q(J_Q) , \qquad (24)$$

where N is the total number of interactions, $Q = 2\pi$, $Q \cdot J_Q(J) = \ln(1 + P/q)$ ($J_Q \sim J$ if $J \to \infty$ or $J \to 0$), and $K(N,J) = e^{-N(2J - QJ_Q)}$.

We are concerned with clusters and spin properties, and in the context of the linear model it is possible to prove a definite relation between correlation g and connectivity c:

$$g(i,j) = e^{-r/\xi} c(i,j) , \qquad (25)$$

where $r = |i - j|$ is the number of spins between S_i and S_j plus one, and

$$\xi^{-1}(J) = \ln[(I_0(J) - e^{-J})/I_1(J)] . \qquad (26)$$

Moreover the connectivity $c(i,j)$ at temperature $T = 1/J$ for the XY model, is equal to the connectivity $c_Q(i,j)$ of the KF (or CK) clusters introduced above in the Q-Potts model with $T = 1/J_Q(J)$ and $Q = 2\pi$:

$$c(i,j)|_J = c_Q(i,j)|_{J_Q(J)} . \qquad (27)$$

These results should shed some light on the connections between cluster connectivity and spin correlation in one-dimensional XY models. A trivial consequence of all these relations in 1D is that $T_p = T_c = 0$ (it would be hard to find clusters with a bit of randomness with $T_p > 0$ in one dimension), but this coincidence does not hold for the critical behavior. Defining ξ_{XY} as the correlation length in the XY model and $\xi_{Q-\text{Potts}}$ as the mean cluster radius in its Q-Potts equivalent, Eq. (25) imposes $\xi_{XY}^{-1} = \xi_{Q-\text{Potts}}^{-1} + \xi^{-1}$, but, in 1D, at low temperature $\xi_{XY} \sim T^{-1}$ while $\xi_{Q-\text{Potts}} \sim e^{A(Q)/T}$ [13,17], and so clusters quite loosely express spin–spin correlations.

6. MC results for the XY model in higher dimensions

The analytical problem concerning the structure of clusters in XY models in higher dimensions, is, worthless to say, much more difficult. We present then some Monte Carlo results about clusters properties (defined from solution (15)), in two and three dimensions.

MC simulations were done using a standard Metropolis spin flip algorithm [18] on n-clock models on a square or cubic lattice described by Hamiltonian (11) (in the following if not specified we will consider the isotropic case $J_{ij} = J \geqslant 0$), whose spin S_i has a phase $\theta_i = 2\pi m/n$ with $m \in \{0, \ldots, n-1\}$.

Let us briefly examine our MC results in two dimensions. In the case $n = 2$ we exactly recover the 2D ferromagnetic Ising model. Our MC simulation indicates the well known result of equal critical temperatures $T_c = T_p = 2.269$ (all temperatures are measured in units of J) and a percolative critical phenomena characterized by Ising exponents. Moreover, the MC dynamics based on the above defined clusters is just the Swendsen-Wang dynamics and the phenomena of critical slowing down drastically reduced [6,7].

For $n > 4$ such correspondence is no longer verified. Such a result may be expected because in these cases connectivity and correlation are not coinciding as shown by the simple example of just two interacting spins with $n = 5$ (the cases $n = 3, 4$ may be successfully faced with some tricks, in resemblance of the possibility to map $n = 3, 4$ clock-models in an equivalent Q-Potts [4]).

The percolation critical temperature decreases for increasing n, and approaches a plateau in the large n limit. In actual facts, via MC simulations, for $n = 36$, we find that the percolation point is at

$$T_p = 1.69 \pm 0.03$$

to be compared with the 2D XY critical temperature at $T_c \sim 0.89$ [7,11]. We find that the percolation critical exponents are in the universality class of random percolation as expected because there is no thermodynamic transition underlying the percolative one: the critical exponents, measured via a finite size scaling analysis [18] (reported in Fig. 1), are $v = 1.33 \pm 0.05$ and $\gamma/v = 1.79 \pm 0.05$ in perfect agreement with 2D random percolation exact values $v = 4/3$ and $\gamma/v = 43/24$. These exponents, in percolation, characterize, respectively, the divergence of mean cluster radius ξ and mean cluster size S: $\xi \sim |T - T_p|^{-v}$ and $S \sim |T - T_p|^{-\gamma}$ [13].

This behavior is observed, as may be easily suspected, in frustrated or disordered systems too. We tested, via MC, the fully frustrated XY model (FF) and the $\pm J$ XY spin glass (SG) (see references in [19]), where we found the same percolative critical exponents and (see the scaling analysis in Figs. 2 and 3):

$$T_p^{\text{FF}} = 1.61 \pm 0.03 \quad \text{and} \quad T_p^{\text{SG}} = 1.64 \pm 0.03 .$$

This value for the percolation transition in the FF model is above the critical region located around $T \sim 0.4$–0.5 (see [19]). Also Wolff's clusters show a percolation point
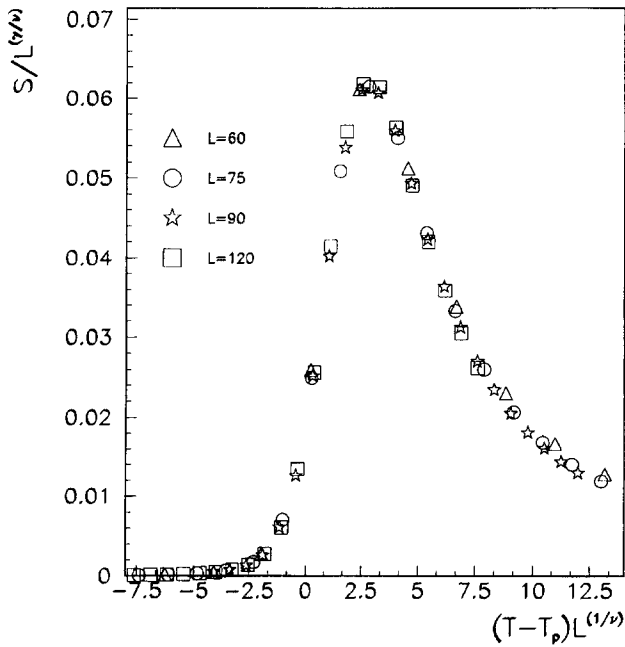
Fig. 1. Finite size scaling of the mean cluster size S defined by bond probabilities given in Eq. (16), in the 2D *XY* ferromagnet. The scaling parameters are $T_p = 1.69 \pm 0.03$ and $v = 1.33 \pm 0.05$, $\gamma/v = 1.79 \pm 0.05$.
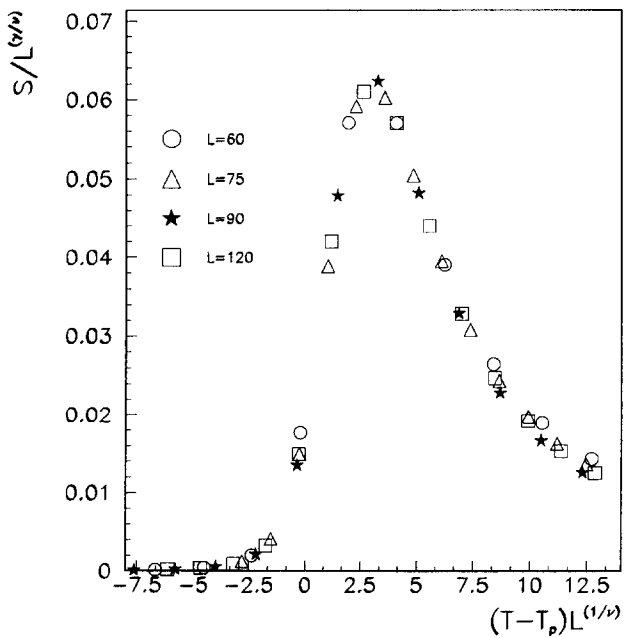

Fig. 2. Finite size scaling of the mean cluster size S of clusters defined by bond probabilities given in Eq. (16), in the 2D *XY* fully frustrated. The scaling parameters are $T_p = 1.61 \pm 0.03$ and $v = 1.33 \pm 0.05$, $\gamma/v = 1.79 \pm 0.05$.
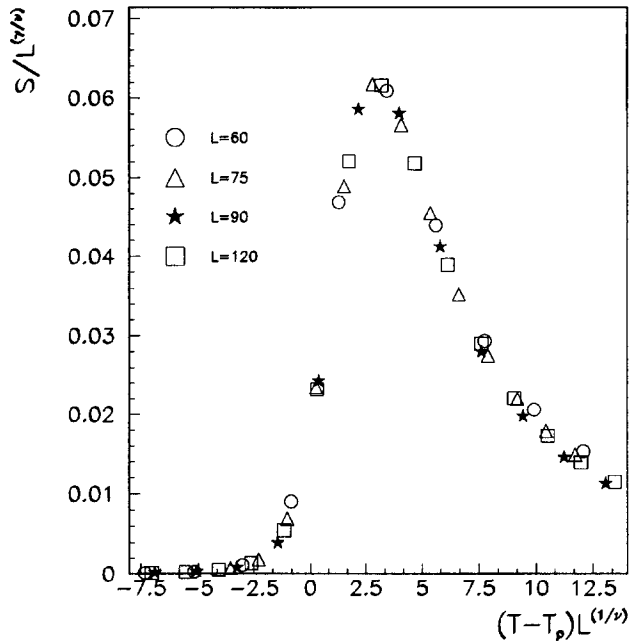
Fig. 3. Finite size scaling of the mean cluster size S of clusters defined by bond probabilities given in Eq. (16), in the 2D XY $\pm J$ spin glass. The scaling parameters are $T_p = 1.64 \pm 0.03$ and $v = 1.33 \pm 0.05$, $\gamma/v = 1.79 \pm 0.05$.
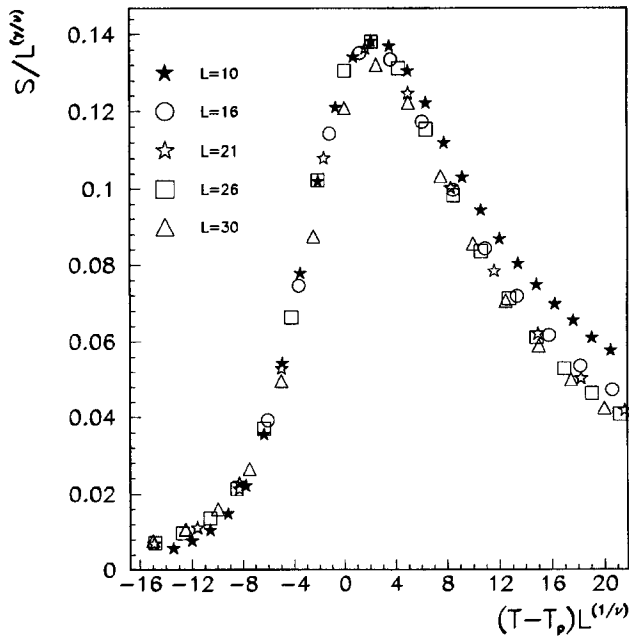

Fig. 4. Finite size scaling of the mean cluster size S of clusters defined by bond probabilities given in Eq. (16), in the 3D XY ferromagnet. The scaling parameters are $T_p = 3.75 \pm 0.05$ and $v = 0.87 \pm 0.05$ $\gamma/v = 2.00 \pm 0.05$

well above the critical region [11], but it is possible to introduce their direct general-
izations whose T_p may be pushed closer and closer to it [20].

The same kind of results are found in three dimensions. For $n = 2$ we recover the
well known properties of KF or SW clusters in the 3D Ising model $T_p = T_c \sim 4.5$ and
$v \sim 0.62$, $\gamma/v \sim 1.97$ (see [21]). Our MC runs show, for $n = 36$, $T_p = 3.75 \pm 0.05$ and
3D random percolation critical behavior with $v = 0.87 \pm 0.05$ and $\gamma/v = 2.00 \pm 0.05$
(see Fig. 4). These values are to be compared to the results of 3D XY $T_c \sim 2.2$ and
$v \sim 0.66$, $\gamma/v \sim 1.98$ (see [22]). Essentially the same values are found for the 3D $\pm J$
XY spin glass.

It is interesting to note that, as expected and discussed above (see also [9,14]),
whenever the gap between T_p and T_c becomes finite, SW like cluster algorithms for
MC simulations are not able to reduce the critical slowing down.

After these MC results, the panorama we get illustrates that the straight generalization
to XY models of KF clusters, given in Eq. (15), does not have the peculiar properties of
KF clusters in Ising like systems: the thermodynamic and percolative transitions are no
longer coincident. In Ising models, more complex procedures have been introduced to
individualize physical clusters, as those proposed in [8,9,14]. It would be interesting to
verify if the extensions to XY of such procedures along the lines proposed above, have
the same percolation properties found here or new interesting results can be obtained.

7. Summary and conclusions

In analogy to the works of Kasteleyn and Fortuin and Coniglio and Klein, clusters of
nearest neighbor spin in XY models may be defined as sets of spin connected by bonds
according definite rules. The clusters divide the original lattice into independent regions
of statistically coherent spins. Kasteleyn and Fortuin's concepts and tools to link clusters
and spin properties, which proved to be so useful in Ising systems, can be extended
to XY models. In these models, at a first simple level, KF clusters may be defined by
separately looking at just each single couple of interacting spins. Consequently, bonds
are introduced between them according to the definite probability distribution given in
Eq. (15) (as a matter of fact, this is for XY models, but the analog for general $O(n)$
is absolutely similar).

Nevertheless, at the simple level here explored, many differences appear with Ising
systems. It is known that in the Ising model these clusters have a percolation point
which, imposing condition (21), may be pushed to coincide with the critical one T_c, and
has percolative exponents in the Ising universality class [1,2]. The properties of the new
clusters may be studied analytically for continuous spin systems in one dimension. Here
Eq. (25) implies that the mean square radius of clusters different from the Ising KF case,
is no longer coincident with the correlation length in the system. Numerical results show
the same behavior in higher dimensions, where moreover cluster percolation point T_p is
different from T_c. Phenomenologically, the temperature T_p is the point where regions of
almost parallel spin (in ferromagnetic models), i.e. regions of coherent spins, percolate

in the system. The transition corresponding to this point, for clusters defined by Eq. (15), is in the random percolation universality class.

The occurrence of a finite gap between T_p and T_c is found in Ising spin systems when frustration is present. In this case a general criterion to close such a gap has been proposed [8,9,14]. Exploiting the results presented here, it is possible to apply such a criterion to frustrated and unfrustrated $O(n)$ models too, and in perspective give a percolative description of their critical behaviors in analogy to the known results for Ising like models. This approach would lead to a change of the bond probability distribution given in Eq. (15). In unfrustrated and frustrated Ising models a definite physical origin has been associated to the percolation point T_p [23]. It is then natural to speculate on it in continuous spin models too.

The criterion introduced in [8,9,14] is actually suited to develop efficient MC cluster algorithms in Ising systems. The perspective to go further in such a direction also for $O(n)$ models, is very appealing.

Acknowledgements

References

[1] P.W. Kasteleyn and C.M. Fortuin, J. Phys. Soc. Japan Suppl. 26 (1969) 11; C.M. Fortuin and P.W. Kasteleyn, Physica (Utrecht) 57 (1972) 536.
[2] A. Coniglio and W. Klein, J. Phys. A 13 (1980) 2775.
[3] M.E. Fisher, Physics (N.Y.) 3 (1967) 225.
[4] F. Wu, Rev. Mod. Phys. 54 (1982) 235.
[5] A. Coniglio, Phys. Rev. Lett. 62 (1989) 3054; A. Coniglio, in: Correlation and Connettivity-Geometric Aspects of Physics, Chemistry and Biology, eds. E. Stanley and W. Ostrowsky, NATO ASI Series, Vol. 188 (1990).
[6] R.H. Swendsen and J.S. Wang, Phys. Rev. Lett. 58 (1987) 86; J.S. Wang and R. Swendsen, Physica A 167 (1990) 565.
[7] U. Wolff, Phys. Rev. Lett. 60 (1988) 1461; U. Wolff, Phys. Rev. Lett. 62 (1989) 361.
[8] D. Kandel, R. Ben-Av and E. Domany, Phys. Rev. Lett. 65 (1990) 941; D. Kandel, R. Ben-Av and E. Domany, Phys. Rev. B 45 (1992) 4700; D. Kandel and E. Domany, Phys. Rev. B 43 (1991) 8539.
[9] V. Cataudella, G. Franzese, M. Nicodemi, A. Scala and A. Coniglio, Phys. Rev. Lett. 72 (1994) 1541; Il Nuovo Cimento D 16 (1995) 1259; Phys. Rev. E 54 (1996) 175.
[10] N. Kawashima and J.E. Gubernatis, Phys. Rev. E 51 (1995) 1547.
[11] P.W. Leung and C.L. Henley, Phys. Rev. B 43 (1991) 752.
[12] A. Coniglio, F. di Liberto, G. Monroy, F. Peruggi, Phys. Rev. B 44 (1991) 12 605.
[13] D. Stauffer and A. Aharony, Introduction to Percolation Theory, 2nd edn. (Taylor and Francis, London, 1995).
[14] M. Nicodemi, J. Phys. A 29 (1996) 1961.
[15] R.G. Edwards and A.D. Sokal, Phys. Rev. D 38 (1988) 2009.
[16] C.S. Hu and S.S. Hsiao, Phisica A 184 (1992) 192.
[17] H.E. Stanley, Phase Transitions and Critical Phenomena (Clarendon Press, Oxford, 1971).
[18] K. Binder, D.W. Hermann, Monte Carlo Simulation in Statistical Physics (Springer, Berlin, 1988).

[19] J. Villain, J. Phys. C 10 (1977) 1771 and 4793; J. Lee, J.M. Kosterlitz and E. Granato, Phys. Rev. B
     43 (1992) 11 531; G. Ramirez-Santiago and J.V. José , Phys. Rev. E 49 (1994) 9567; P. Olson, Phys.
     Rev. Lett. 75 (1995) 2758.
[20] V. Cataudella and M. Nicodemi, Physica A 233 (1996) 293.
[21] A.M. Ferrenberg and D.P. Landau, Phys. Rev. B 44 (1991) 5081.
[22] A.P. Gottlob and M. Hasenbusch, Physica A 201 (1993) 593.
[23] See references: in A. Coniglio, Il Nuovo Cimento 16D (1994) 1027; and the Proc. of the Euroconference
     on Non-equilibrium Phenomena in Supercooled Fluids, Glasses and Amorphous Materials, Pisa (1995).