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LETTER TO THE EDITOR

Exact relations between droplets and thermal fluctuations in external field

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Abstract. We extend the definition of droplets in Ising and Potts models to the case of an external field different from zero. We also find exact relations between thermal properties and connectivity properties which show why, in mean field, the mean cluster size does not diverge as the susceptibility when the critical temperature is approached from below.

How to describe a critical fluctuation near a critical point is an old problem which has received much attention [1-9]. In a ferromagnetic Ising model, for example, it is well known that the clusters made of nearest-neighbour spins in the same state are not suitable for the description of the phase transition at the critical point because they either diverge at temperatures higher than the critical temperature, or diverge at the critical temperature with percolative critical exponents different from the thermal ones. To properly describe the fluctuation, another definition of cluster (called droplet) was proposed for the ferromagnetic Ising model [5], and generalised later to the Potts model and to the antiferromagnetic Ising model [3,10]. The droplets are defined as those clusters such that any pair of spins is connected through a chain of parallel spins and active bonds. A bond is active with probability $p_B = 1 - e^{2J}$ or non-active with probability $q_B = 1 - p_B$. Here J is the nearest-neighbour pair interaction of the Ising model, whose Hamiltonian has the standard form:

$$-\beta H = J \sum_{\langle ij \rangle} s_i s_j + H \sum_i s_i. \tag{1}$$

More specifically the droplet model is defined as a site-bond correlated percolation problem: in the Ising model the sites exhibit the usual correlations, while the bonds are allowed to be in two states, active or nonactive, which are assumed independently from those of the other bonds and from spin configurations. The droplet model describes correctly the thermal phase transition in terms of the percolative transitions undergone by the droplets at the critical point, where both percolation exponents and thermal exponents coincide [5]. Although the droplet picture clarifies the behaviour of the Ising model allowing a geometric interpretation in terms of clusters, its full validity is, however, limited to the $H = 0$, $T > T_c$ region. Extending naively the model to $H > 0$, for example, one finds that there exists a spurious percolative critical line which starts from the critical point and separates the low-temperature percolative region from the high-temperature non-percolative region, although it is well known

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that there are no thermal transitions in the presence of the field. Moreover, in mean-field theory it has never been clear why, even at $H=0$, the mean droplet size does not diverge with the same critical exponent as the susceptibility [11, 12], when T_c is approached from below.

Recently Swendsen and Wang [13] introduced a new dynamics, which instead of flipping one spin at a time, flips altogether all the spins in the same droplet. The resulting algorithm has proved to be extremely fast compared with the Glauber dynamics, with a drastic reduction of the critical slowing down. How to elaborate the Swendsen-Wang dynamics to further reduce the critical slowing down is a big open question which may be enlightened by a precise relation between droplets and thermal properties.

In this letter, following Kasteleyn and Fortuin [3] and Swendsen and Wang [13], we introduce a ghost-spin approach which allows us to extend properly the definition of the droplets to $H \neq 0$. We obtain some exact relations between thermal and connectivity properties, valid for every H and T. Using these relations we will also be able to explain why, in mean field, the susceptibility and the mean droplet size do not coincide at $H=0$, $T \to T_c^-$.

We start from the Hamiltonian (1), where it is understood that the sums over i and $\langle ij \rangle$ are extended, respectively, to the set V of sites and to the set E of bonds of a lattice. We define an extended lattice adding to the 'real' lattice a 'ghost' site connected to each site of the 'real' lattice by means of a 'ghost' bond. Assuming that the ghost site is occupied by a spin (fixed in the up state for $H>0$, and fixed in the down state for $H<0$), we can treat the magnetic field on the real lattice as a further nearest-neighbour interaction on the extended lattice. Therefore, in complete analogy with real bonds, we consider a ghost bond active with probability $p_G = 1 - e^{-|H|}$, and non-active with probability $q_G = 1 - p_G$. The droplets are still defined as above, but now the connectivity can be realised also through the ghost site (see figure 1). As a first result we observe that, for $H>0$, infinitely many up spins connect with the ghost site, giving rise to an infinite droplet at every temperature. The same happens for $H<0$ and down droplets: thus the spurious percolation critical lines at $H \neq 0$ are no longer present. It is also easy to prove that any infinite droplet is always connected to the ghost spin. As a byproduct we also have that any droplet disconnected from the ghost is finite.

Now, in order to describe explicitly the relations between thermal and percolative functions, we give our main quantitative results. Both the expected values of thermal and percolative functions f, will be evaluated making use of the following average:

$$\langle f \rangle = \frac{\sum_{\{s\}} e^{-\beta H} \sum_{C_s \subseteq \hat{E}_s} f p^{C_s} q^{\hat{E}_s - C_s}}{\sum_{\{s\}} e^{-\beta H} \sum_{C_s \subseteq \hat{E}_s} p^{C_s} q^{\hat{E}_s - C_s}} . \tag{2}$$

Here $\{s\}$ is any spin configuration of the real lattice (remember that the ghost spin is always in the fixed state $s_0 = H/|H|$, the zero-field case being recovered in the limits $H \to 0^+$); $\hat{E}_s$ is the set of all real and ghost bonds connecting parallel spins in the configuration $(\{s\}, s_0)$ of the extended lattice; $p^{C_s} = \Pi_{\langle ij \rangle \in C_s} p_{ij}$; and $p_{ij} = p_B$ if $\langle ij \rangle$ is a real bond, or $p_{ij} = p_G$ if $\langle ij \rangle$ is a ghost bond. Note that expression (2) reduces to the usual droplet average simply substituting $\hat{E}_s$ with the set E_s of all real bonds connecting parallel spins in the configuration $\{s\}$ of the real lattice. Also note that for simplicity we refer to both clusters of up and down spins as droplets, although we can always distinguish among up and down droplets, if necessary. Finally, remark that when the average (2) is applied to a thermal function $f = f(\{s\})$, it reduces to the usual thermal

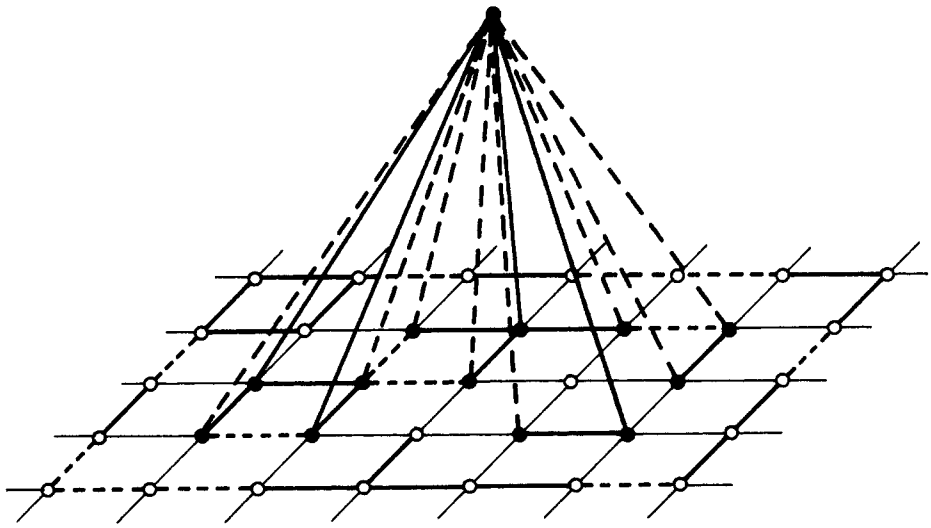

Figure 1. A configuration of the Ising model in external field on the square lattice is shown. Up (down) spins are represented by closed (open) circles; nearest-neighbour spins in the same state are connected by active bonds (lines) or disconnected by non-active bonds (broken lines). Three up droplets on the lattice are connected together (and to the infinite up droplet) through the ghost site; a fourth up droplet is disconnected from the ghost site and thus remains finite.

average, because

$$\sum_{C_s \subseteq \hat{E}_s} p^{C_s} q^{\hat{E}_s - C_s} = 1. \tag{3}$$

While our previous works were based on an indirect argument suggesting the relation between thermal and percolative functions, we have now also proved such a relation in a direct way. The result is that, given any (thermal) function $f(\{s\})$, the (percolative) function $g(C_s)$ which satisfies

$$\langle f(\{s\})\rangle = \langle g(C_s)\rangle \tag{4}$$

is given by

$$g(C_s) = \frac{\Sigma_{\{s\}} f(\{s\})\delta(C_s)}{2^{N(C_s)}}. \tag{5}$$

Here $\delta(C_s)$ is an indicator which equals 1 if in the spin configuration $\{s\}$ one has $s_i = s_j$ for every $\langle ij\rangle \in C_s$, and is 0 otherwise, while $N(C_s)$ is the number of finite droplets in the configuration C_s. Applying relation (5) to the thermal functions s_i and $s_i s_j$, and making use of (4), it is possible to show that in the thermodynamic limit one has

$$\langle s_i\rangle = (H/|H|) < \gamma_i^{\inf}\rangle \tag{6}$$

$$\langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle = \langle \gamma_{ij}^{f+}\rangle + \langle \gamma_{ij}^{f-}\rangle + (<\gamma_i^{\inf}\gamma_j^{\inf}\rangle - \langle \gamma_i^{\inf}\rangle\langle \gamma_j^{\inf}\rangle) \tag{7}$$

where $\gamma_i^{\inf}(C_s)$ is an indicator which assumes the value 1 if the site i is connected (also not directly) to the ghost spin, and is 0 otherwise, while $\gamma_{ij}^{f+}(C_s)$ ($\gamma_{ij}^{f-}(C_s)$) is 1 if i and j belong to the same finite up (down) droplet, and is 0 therwise. If one writes

down the functions corresponding to the averages in relations (6) and (7) they assume the following form:

$$M = \frac{H}{|H|}\rho^{\inf} = \begin{cases} \rho^{+}P^{+} & \text{if } H > 0 \\ \rho^{-}P^{-} & \text{if } H > 0 \end{cases} \tag{8}$$

$$G_{ij} = P_{ij}^{+} + P_{ij}^{-} + [\langle \gamma_i^{\inf}\gamma_j^{\inf}\rangle - (\rho^{\inf})^2]. \tag{9}$$

Thus we have obtained an expression of the magnetisation M in terms of the density $\rho^{\inf}$ of sites belonging to the infinite droplet, i.e. in terms of the density ρ^{+} (ρ^{-}) of up (down) spins and the percolation probability P^{+} (P^{-}) for up (down) spins. Equation (9), instead, relates the correlation function G_{ij} to the pair connectedness P_{ij}^{+}, (P_{ij}^{-}) for up (down) spins and to the term between brackets, which can be interpreted as a fluctuation of the infinite droplet. Observe that, since the magnetisation is defined as $M = \rho^{+} - \rho^{-}$, relation (8) implies that the density of sites belonging to finite droplets of up spins is equal to the density of sites belonging to finite droplets of down spins for every H and T. Furthermore, summing (9) over all sites, and taking into account the fact that $\chi = \Sigma G_{ij}$ and $S^{+} = \Sigma P_{ij}^{+}$ ($S_{-} = \Sigma P_{ij}^{-}$), we obtain a relation between the susceptibility and the mean size of finite droplets:

$$\chi = S^{+} + S^{+}X^{\inf} \tag{10}$$

where the last term arises from the fluctuations of the infinite droplet. This relation was originally found [14] for $H = 0$ and very recently has been obtained independently [15]. We emphasise that relations (6)-(10) hold everywhere in the H, T plane. Therefore, from (9) we deduce that $G_{ij} = P_{ij}^{+} + P_{ij}^{-}$ only if the infinite droplet is not present, namely, from (8), if the magnetisation is zero. Therefore the exact coincidence of mean cluster size and susceptibility holds exactly only when $M = 0$. This explains why in mean field for $H = 0$ and $T \to T_c^{-}$ the mean cluster size diverges with an exponent different from that of the susceptibility. For $d = 2$ numerical calculations [14] indicate that they diverge in the same way although the rate of the amplitude of the mean cluster size above and below T_c is different from that related to the susceptibility. We expect that this should be true for all dimension up to $d = 4$, since $d = 4$ is the upper critical dimension for the Ising model, while for percolation the upper critical dimension is $d = 6$.

Another property characterises mean-field theories, namely the existence of metastable phases with magnetisation opposite to the field, which appear in a region around the $H = 0$, $T < T_c$ line. This region is delimited by spinodal lines where the susceptibility of the metastable phase diverges. To describe correctly the problem in terms of the droplets defined here, one must take into account the coexistence of infinite droplets of up and down spins. For example, in the metastable phase at $H > 0$, due to the down magnetisation, we have an infinite droplet of down spins disconnected from the ghost site, but also an infinite droplet of up spins made of infinitely many finite droplets connected through the ghost site. We have shown that our previous formulae can be extended to this case, too; for example, the general form of relations (8) and (10) is

$$M = \rho^{\inf+} - \rho^{\inf-} \tag{11}$$

$$\chi = S^{+} + S^{-} + X^{\inf+} + X^{\inf-}. \tag{12}$$

In the Bethe lattice model and in mean field we have verified equations (11) and (12). We have also found that along the spinodal line, where the susceptibility diverges, the mean droplet size $S^{+} + S^{-}$ stays finite. Therefore this type of droplet is not suitable

to describe nucleation in a mean-field theory. In fact one can use a different approach and choose $p_G = 0$ and p_B in such a way that the mean cluster size and the susceptibility diverge along the same line. Such a choice gives in mean field [16] a value $p_B = 1 - \exp[-2J(1-M^2)]$.

We report now a brief discussion about the connections of the present droplet model and the well established formalism of Kasteleyn and Fortuin (KF). From the average definition (2), summing over all spin variables, it can be proven that for every percolative function $f(C_s)$:

$$\langle f(C_s)\rangle = \langle f(C)\rangle_{KF} = \frac{\Sigma_{C\subseteq\hat{E}} f(C) p^C q^{\hat{E}-C} 2^{N(C)}}{\Sigma_{C\subseteq\hat{E}} p^C q^{\hat{E}-C} 2^{N(C)}}. \tag{13}$$

All the quantities appearing in the KF average have been already defined in the droplet approach, the only difference being in the fact that the KF average is performed in a pure bond percolation context. Indeed the memory of spin configurations is completely lost, because $\hat{E}$ is the set of all bonds of the extended lattice and does not depend on $\{s\}$, while $N(C)$ is the number of clusters in the bond configuration C. The interest of the KF average lies in the fact that the expectation values of the relevant percolative functions are equal to those of some related thermal functions; e.g. one has the relation:

$$\langle s_i s_j\rangle_{\text{therm}} = \langle \gamma_{ij}\rangle_{KF} \tag{14}$$

where $\gamma_{ij}(C)$ is 1 if i and j belong to the same cluster, and 0 otherwise. With respect to the KF relations, the droplet approach has the advantage that both thermal and percolative functions are evaluated with the same average, rather than in two different contexts. As stressed by Hu [8], the KF average (10) can also be interpreted in terms of a bond-correlated percolation model (the interactions between bonds being implied by the weight $2^{N(C)}$). However, we think that the substitution of site correlations with bond correlations masks the intuitive picture of the spin model that one would gain in terms of percolation. Indeed, the distinctive aspect of our droplet picture (which is a correlated-site and random-bond percolation model) lies in the fact that the spins are still present in the cluster definition, while the bonds are used to separate and/or connect them in such a way to give the cluster definition which correctly reproduces the thermal behaviour.

Complete details about our method, its extension to the ferromagnetic Potts model, and exact calculations on the Bethe lattice and in mean-field theory will be given in a forthcoming paper.

In conclusion, the droplet picture gives a good description of the thermal fluctuation whenever the magnetisation is zero. When the magnetisation is different from zero we distinguish two contributions to the thermal fluctuation: one is due to the finite droplets, the second is due to the fluctuation of the infinite droplet (see (9)). It would be interesting to investigate whether it is this non-exact equivalence of thermal fluctuations and finite droplets that induces a non-zero critical slowing down in the Swendesn–Wang dynamics. If one wants to define thermal fluctuations in terms only of finite geometrical clusters, one needs a different definition of the droplet. A suggestion toward the solution of this problem, at least in mean field theory, has been made by Wang [15].

Note added. After this paper was completed three preprints, by Wang [17], Kertesz [18] and Alexandrowicz [19], have circulated concerning the definition of droplets in an external magnetic field.

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