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Cluster approach to spin glasses and the frustrated-percolation problem

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Exact relations between cluster properties and thermodynamical properties are obtained for an Ising spin glass. The size of the clusters diverges at a temperature higher than the spin-glass transition. The clusters represent fluctuations that interfere with each other giving rise to net correlations of much shorter size than the typical cluster radius. A frustrated-percolation model is introduced that is related to the Ising spin glass as standard percolation is related to the Ising model.

The description of fluctuations in terms of geometrical clusters has been the object of intensive study for many years.[1–8] It is well known[2] that in an Ising model the naïve definition of clusters made of nearest-neighbor (NN) parallel spins is not satisfactory to describe the correlations. Such clusters are present even at infinite temperature where the correlations are zero. A more convenient definition of a cluster (also called droplet) was given[4] for the NN Ising model with zero external field by introducing bonds between NN parallel spins, each bond being present with probability p given by

$$p = 1 - e^{-2J/kT} , \tag{1}$$

where J is the NN spin interaction. Two spins belong to the same cluster if they are connected by at least one chain of bonds. Using a Hamiltonian formalism based on a dilute Potts model it is possible to show[4] that the size of these droplets diverges at the Ising critical point with Ising exponents and therefore they represent regions of correlated spins. These results were generalized[5] later to the q-state Potts model. More recently a more direct approach[9] enabled us to establish exact relations between connectivity properties and thermodynamical properties without using the dilute Hamiltonian formalism. These clusters, that are related to the Kasteleyn-Fortuin formalism[3] of the q-state Potts model, have been employed by Swendsen and Wang[10,11] (SW) to develop a cluster dynamics which has the property of reducing drastically the critical slowing down. This dynamics flips in one step all the spins in the same cluster without having to wait for the correlation to propagate. In this paper we want to extend the above definition of a cluster[12] to the Ising spin-glass and relate their connectivity to the thermodynamical properties. It will be shown that these clusters represent interfering fluctuations that reduce the spin-spin correlations to a range much shorter than the typical cluster size. This result explains why the SW dynamics, as it stands now, is not efficient in the spin-glass problem[11] even though it is in the Ising case. The size of the clusters diverges at a temperature T_p higher than the spin-glass temperature T_{SG}. The possible presence of a singularity in the free energy at T_p is discussed. By developing the cluster formalism, we will also introduce a frustrated-percolation model that is related to the Ising spin-glass as ordinary percolation is related to the pure ferromagnetic Ising model.

Before we consider the spin-glass case, it is convenient to recall briefly the cluster formalism and its connection to the thermodynamical properties for the pure Ising model. Following a recent approach[9] we consider the NN Ising Hamiltonian in the following form:

$$-H = J \sum_{\langle i,j \rangle} (s_i s_j - 1) , \tag{2}$$

where $s_i = \pm 1$. For any configuration of spins we introduce bonds only between NN pairs of parallel spins with probability given by (1). The weight $W(\{s_i\}, C)$ for a given configuration of spins $\{s_i\}$ and bonds C is given by

$$W(\{s_i\}, C) = p^{|C|}(1-p)^{|B|} e^{-H/kT} , \tag{3}$$

where $|C|$ is the number of bonds in the configuration C, and $|B|$ the number of absent bonds between parallel spins. From the Hamiltonian (2) $e^{-H/kT} = (e^{-2J/kT})^{|D|}$, where $|D|$ is the number of NN pairs of antiparallel spins. Using (2), the weight (3) can be written in the following way:

$$W(\{s_i\}, C) = p^{|C|}(1-p)^{|A|} \prod_{\langle i,j \rangle \in C} \delta_{s_i s_j} , \tag{4}$$

where $|A| = |B| + |D|$ is the total number of absent bonds. The product over the Kroenecker delta $\delta_{s_i s_j}$ takes into account the condition that the bonds $\langle i,j \rangle$ in the configuration C are present only between parallel spins; otherwise the weight is zero.

It is possible to prove the following relations, using (4):[3,9]

$$\langle s_i \rangle = \langle \gamma_i^{\rm inf} \rangle, \quad \langle s_i s_j \rangle = \langle \gamma_{ij} \rangle , \tag{5}$$

where $\gamma_i^{\rm inf} = 1$ or 0 depending whether or not site i belongs to the infinite cluster and $\gamma_{ij} = 1$ or 0 depending whether or not i and j are in the same cluster, $m_i \equiv$

$\langle s_i \rangle$ is the magnetization at site i, $P_i \equiv \langle \gamma_i^{\inf} \rangle$ is the probability that site i belongs to an infinite cluster (for a system of infinite size these quantities are independent on i), and $p_{ij} \equiv \langle \gamma_{ij} \rangle$ is the probability that i and j are in the same cluster; $\langle ... \rangle = \sum ... W(C, \{s_i\})/Z$ stands for the average over all spin and bond configurations with weight given by (4).

The partition function Z can formally be written in two ways. By taking first the sum of (3) over the allowed bond configurations, we have the usual expression $Z = \sum_{\{s_i\}} e^{-H/kT}$. Alternatively from (4), taking first the sum over the spin configurations, Z can be expressed in the Kasteleyn and Fortuin formalism:

$$Z = \sum_C p^{|C|}(1-p)^{|A|} q^{N(C)} . \qquad (6)$$

Here $q = 2$ and $q^{N(C)}$ is the number of configurations of spins compatible with the bond configuration C and $N(C)$ is the number of clusters in the bond configuration C. For any value of q in (6) one obtains the partition function for the q-state Potts model.

From (5) it follows that the magnetization and the percolation probability go to zero at the same point. Therefore the Ising critical point and the percolation point of the clusters coincide.

We now show how to extend the cluster definition and their relations to the thermodynamical quantities for the Ising spin-glass model.[13] We consider the NN Ising-spin-glass Hamiltonian in the following form:

$$-H = \sum_{\langle i,j \rangle} (J_{ij} s_i s_j - | J_{ij} |) , \qquad (7)$$

where the NN interaction $J_{ij} = \pm J$ are randomly distributed and the constant in the Hamiltonian has been chosen for convenience in such a way that the energy between two spins satisfying the interaction is zero and $-2J$ if they do not. A concept crucial in spin glasses is frustration. Frustration occurs when for a given realization of interactions it is impossible for all the spins to satisfy at the same time their mutual interactions so that $J_{ij} s_i s_j > 0$. Frustration occurs if and only if there is at least one loop which contains an odd number of interactions. For a fixed configuration of interactions the average magnetization at site i is given by $m_i = \langle s_i \rangle_J$, where $\langle ... \rangle_J$ stands for the thermal average for a fixed configuration of interactions $\{J_{ij}\}$. For high temperatures $m_i = 0$. For low temperatures the spin-glass phase is characterized by the Edward-Anderson order parameter: $q_{\text{EA}} = \frac{1}{\mathcal{N}} \sum_i \overline{\langle s_i \rangle_J^2}$, where $\mathcal{N}$ is the number of spins and the bar stands for the average over all the interaction configurations. q_{EA} is different from zero in the spin glass phase and goes to zero at the spin-glass temperature T_{SG}. Similarly one defines the pair correlation function: $g_{ij} = \langle s_i s_j \rangle_J - \langle s_i \rangle_J \langle s_j \rangle_J$. However, since the sites can be positively and negatively correlated, one defines more appropriately $C_{ij} = \overline{g_{ij}^2}$, which is related to the Edward-Anderson susceptibility, $\chi_{\text{EA}} = \sum_j C_{ij}$. This quantity diverges at T_{SG} and remains divergent for all temperatures below T_{SG}.

In the Ising spin glass, for a given realization of interactions $\{J_{i,j}\}$ and a given configuration of spins, the clusters are defined by putting bonds only between those pairs of spins that satisfy the interaction $J_{ij} s_i s_j > 0$, the bond probability being given by (1). Two spins are in the same cluster if they are connected by at least one chain of bonds. (See Fig. 1.) Following the previous formalism the weight for each configuration of spins $\{s_i\}$ and bond C can be shown to be given by

$$W(\{s_i\}, C) = p^{|C|}(1-p)^{|A|} \prod_{(i,j) \in C_F} \delta_{\sigma_i \sigma_j} \prod_{(m,n) \in C_A} (1 - \delta_{\sigma_m \sigma_n}) . \qquad (8)$$

As in (4) $| A |$ is the total number of absent bonds, C_F and C_A are the subsets of C made of bonds present on top, respectively, of ferromagnetic and antiferromagnetic interactions. The double product takes into account the fact that the weight (8) is zero whenever the bonds in C are not inserted between spins satisfying the interaction. As a consequence those sets of bonds C which contain a frustrated loop have always zero weight since there is never a configuration of spins which can be consistent with such bonds. Following the same procedure as for the ferromagnetic Ising model, it is straightforward to prove the following relations:

$$\langle s_i \rangle_J = \langle \gamma_{i\uparrow}^{\inf} \rangle_J - \langle \gamma_{i\downarrow}^{\inf} \rangle_J , \qquad (9)$$

$$\langle s_i s_j \rangle_J = \langle \gamma_{ij\parallel} \rangle_J - \langle \gamma_{ij\nparallel} \rangle_J , \qquad (10)$$

where $\gamma_{i\uparrow}^{\inf}$ $(\gamma_{i\downarrow}^{\inf})$ is 1 or 0 depending whether or not site i is up (down) and belongs to the infinite cluster; $\gamma_{ij\parallel}$ $(\gamma_{ij\nparallel})$ is 0 or 1 depending whether or not i and j are parallel (antiparallel) and belong to the same cluster; $P_{i\uparrow} \equiv \langle \gamma_{i\uparrow}^{\inf} \rangle_J$ $(P_{i\downarrow} \equiv \langle \gamma_{i\downarrow}^{\inf} \rangle)$ is the probability that i is up (down) and belongs to the infinite cluster and $p_{ij\parallel} \equiv \langle \gamma_{ij\parallel} \rangle_J$ $(p_{ij\nparallel} \equiv \langle \gamma_{ij\nparallel} \rangle_J)$ is the probability that the spins i and j are parallel (antiparallel) and belong to the same cluster. The angular brackets stand for an average over all configurations of spins $\{s_i\}$ and bonds C with weight given by (8).

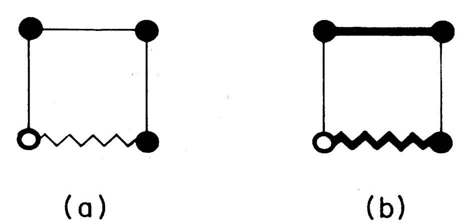

FIG. 1. (a) Example of a configuration of *up* and *down* spins, represented, respectively, by filled and empty circles. Straight and wavy lines indicate ferromagnetic and antiferromagnetic interactions, respectively. (b) Clusters obtained from the configuration given in (a) by putting bonds (heavy lines) between spins satisfying the interaction with a probability p given in Eq. (1).

As for the Ising ferromagnetic case, the partition function for a given realization $\{J_{ij}\}$ can be written in the standard way, $Z(\{J_{ij}\}) = \sum_{\{s_i\}} e^{-H/kT}$; or otherwise, by summing (8) over the spin configurations first Z can also be written

$$Z(\{J_{ij}\}) = \sum_{C}{}^{\star}\, p^{|C|}(1-p)^{|A|} q^{N(C)}, \tag{11}$$

where $q = 2$ and the star means that the sum must be taken only over those configurations C that do not contain frustration.

We note that in contrast to the ferromagnetic case, the thermal quantities are related to differences of connectivity quantities. Therefore $m_i = 0$ (namely $q_{\rm EA} = 0$) implies $P_{i\uparrow} = P_{i\downarrow}$, but it does not necessarily imply $P_{i\uparrow} = P_{i\downarrow} = 0$. Consequently the density of sites in the infinite cluster

$$\rho^{\rm inf} = \frac{1}{\mathcal{N}} \sum_i (P_{i\uparrow} + P_{i\downarrow}) \tag{12}$$

can go to zero at a percolation temperature $T_p > T_{\rm SG}$. For example, for the cubic lattice, with $J/K = 1$, recent numerical calculations[14] showed that such percolation temperature occurs at a value $T_p \simeq 3.92$ below the critical temperature of the pure Ising model $T_c \simeq 4.5$ and well above the spin-glass transition $T_{\rm SG} \simeq 1.2$, with critical exponents numerically indistinguishable from random percolation exponents.

Since the size of the clusters does not diverge at the spin-glass transition, they no longer represent correlated regions of spins. What is their physical meaning? One can still consider these clusters as fluctuations that contribute to the correlations as in the pure ferromagnetic Ising model. However, in the ferromagnetic case, two spins i and j that belong to the same cluster have always the same relative orientation: either both up or both down. Therefore if the spin i is fixed to be up, j is also fixed to be up, and this gives rise to a net correlation between i and j. In the spin glass, we can have two distinct clusters with i up and j up in one cluster and i still up and j down in the other cluster (see Fig. 2). Therefore although both clusters can be viewed as fluctuations that can arise in the system, these fluctuations can interfere. Due to this interference effect the net correlation is greatly reduced compared to the average size of the clusters. For this reason the cluster size does not coincide with the size of the correlated region.

Does the percolation transition correspond to a singularity in the free energy? This is certainly the case for the ferromagnetic Ising model where the critical temperature and the percolation temperature coincide, $T_c = T_p$. A direct evidence of such singularity at T_p can be found in the particular formulation of the partition function (6), expressed in terms of the cluster number $N(C)$. Since at the percolation temperature T_p the cluster number is singular, it follows that the free energy must also contain this singularity.

In the spin-glass case, using the cluster formulation, we have written the partition function in a similar way (11), and by the same argument the free energy should

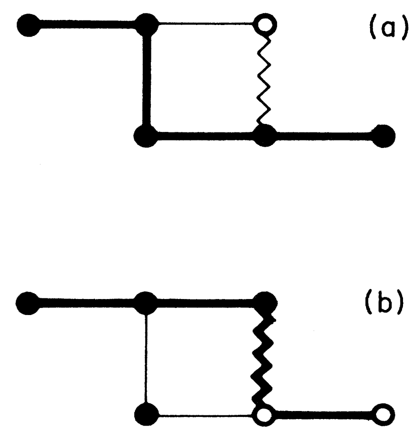

FIG. 2. Clusters contributing to correlations. In both clusters site i is sending signals to site j. The signals, however, have opposite sign and the effect is null.

also have a singularity at the percolation temperature T_p. However, this singularity would disappear if the singular part of the free energy contains a prefactor $Q-2$. Numerical work is under way to investigate the existence and the nature of this singularity.[15]

Frustrated percolation model. Finally we discuss the partition function (11) with $q \neq 2$. Unlike the corresponding pure ferromagnetic case other values of q do not give the partition function of the spin-glass q-state Potts model. However, it is still of interest to extend (11) to all values of q. As a special case in the limit $q = 1$ we obtain what we call the "frustrated-percolation model." This is defined in the following way: For any given configuration of interactions $\{J_{ij}\}$ and for a fixed value of p, a bond configuration C which does not contain frustration has a weight given by

$$W(C) = p^{|C|}(1-p)^{|A|}\ , \tag{13}$$

while those bond configurations which contain frustration have zero weight. This is a percolation problem which is related to the spin-glass model in the same way as standard percolation[16] is related to the Ising model. For $p = 0$ there are only one-site clusters. For $p \to 1$ the ground states are obtained by maximizing the number of bonds in the lattice with the constraint that the bond configuration does not contain frustration. To stress more explicitly the analogy with the Ising spin glass we map a value of p with a temperature given by (1) and each configuration of bonds with a configuration of spins obtained by fixing at random in each cluster one of the two configurations of spins which satisfy the interaction in that cluster.[17] (See Fig. 3.) It is easy to realize that the ground states at $T = 0$ $(p = 1)$ and the disordered state at $T = \infty$ $(p = 0)$ coincide with those of the Ising spin glass. For intermediate values of T we expect a behavior similar to that of the Ising spin glass, with a spin-glass transition temperature and a percolation temperature. As for the dilute quenched Ising ferromagnet, it can be shown that the free energy $F = \langle N(C)\rangle \ln 2$, where $\langle N(C)\rangle$ is the average number of clusters in the

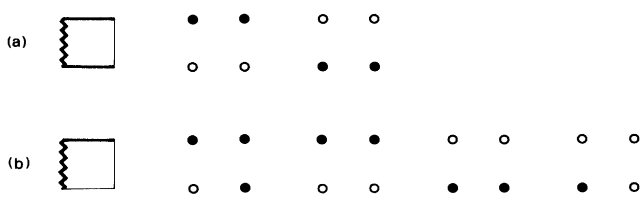

FIG. 3. Example of configurations made of three bonds with weight $p^3(1-p)$ (a) and two bonds with weight $p^2(1-p)^2$ (b). Straight and wavy lines represent positive and negative interactions, respectively; heavy lines indicate the presence of bonds. There is no allowed configuration of four bonds since in this case it would necessarily contain the frustrated plaquette. For each configuration of bonds, also shown is the set of all spin configurations obtained by fixing at random in each cluster one of the two spin configurations which satisfy the interaction in that cluster.

frustrated-percolation problem. Therefore the free energy has a singularity at T_p identical to that of the average number of clusters.

The advantage of studying the frustrated-percolation problem is that it is essentially a geometrical problem and as in percolation there is no slowing down. However, the main problem consists in implementing an efficient algorithm to generate the bond configurations that do not contain frustration.

Another interesting case is the limit $q \to 0$ which describes tree percolation.[18] In this problem the only configurations are those without loops. Since these configurations do not contain frustration, the cluster distribution and the percolation properties are the same as for standard tree percolation. However, by introducing the spin variables as described before one can calculate other quantities typical of a spin glass. In principle one can also calculate deviations from the tree problem by introducing one or more loops into the problem in a systematic way.

In conclusion we have presented exact relations between cluster properties and thermodynamical properties in a Ising spin glass. These clusters, which represent fluctuations of spins unlike the Ising model, interfere and give rise to spin correlations with a range much shorter than the typical cluster size. This property explains why the Swendsen and Wang dynamics is not so efficient as in the Ising case. An efficient dynamics should introduce a way to break further apart the clusters[19] so that the cluster size coincides with the correlated region of spins. Finally we note that, while the clusters in the Ising model well represent the droplets introduced by Fisher[1] to describe the behavior near critical points, the analogous clusters introduced here for the spin glasses should not be confused with the droplets introduced by Fisher and Huse,[20] which describe the critical behavior at the spin-glass transition.

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