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CLUSTERS AND FRACTALS IN THE ISING SPIN GLASS

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Abstract

We define clusters in the Ising $\pm J$ spin glass model, and present evidence for a percolation transition of these correlated clusters coincident with the thermodynamic transition. At the transition temperature T_{sg}, we search for the appropriate clusters of quasifrozen spins which will percolate with exponents in the Ising spin glass universality class. These clusters should provide the dominant contribution to the nonlinear susceptibility, which diverges at T_{sg}, and result from the interference of clusters of parallel and antiparallel spins, as predicted by the Frustrated Percolation model.

Clusters play a central role in describing the purely geometric transition observed in random percolation. Consider the case of random site percolation on a lattice. Place a bond between all sites which are occupied and are also nearest neighbors. A cluster is the set of connected sites. Following the earlier ideas of Fisher,[1] one postulates that the number of clusters of size s, n_s is:

$$n_s \propto s^{-\tau} F((p - p_c)s^{\sigma}), \tag{1}$$

τ and σ are critical exponents which determine the universality class of the system, p_c the percolation threshold. The critical exponents describing the divergence of quantities such as the mean cluster size, etc. are all expressed in terms of τ and σ.[2] The fractal dimensionality,[3] d_f of the spanning cluster at the percolation threshold, p_c is found from scaling to be:

$$d_f = d(1 - (\tau - 1)/(\tau - 1)). \tag{2}$$

Cluster descriptions of thermodynamic phase transitions have elucidated the nature of the transitions by providing a geometrical interpretation of thermodynamic correlations. In particular, the second order thermodynamic transition in the Ising model was explained in terms of clusters by Coniglio and Klein[4] (CK) in 1979. They showed that nearest-neighbor parallel spins connected by fictitious bonds percolated at the transition temperature T_c, with exponents in the Ising universality class. Previously, it had been suggested that the relevant clusters which diverged at T_c should simply be clusters of nearest-neighbor parallel spins, similar to percolation. However, it was soon discovered that these clusters so defined diverged at a temperature higher than T_c (except in $d = 2$), and with exponents in the universality class of random percolation, rather than the Ising universality class. Furthermore, the fractal dimensionality of this spanning cluster is not the same as that expected from scaling arguments for the Ising model at its critical point. Coniglio and Klein showed that by throwing bonds between nearest-neighbor pairs of parallel spins (i.e., spins that satisfy the ferromagnetic interaction) with a probability

$$p_b = 1 - \exp(-2J/k_B T), \tag{3}$$

one obtains a subset of spins that percolate at the Ising transition, and with Ising exponents. Thus this particular choice of bond probability results, in the case of the Ising model, in an equality between the pair correlation function $g_{ij} \equiv \langle S_i S_j \rangle$ and the pair-connectedness function p_{ij}:

$$g_{ij} = p_{ij}, \tag{4}$$

where p_{ij} is the probability that sites i and j are connected by at least one path of bonds (i.e., that they belong to the same cluster). Consequently, the diverging correlation length corresponding to the susceptibility can be understood in terms of diverging connectivity.

Using the CK prescription, the Ising model can be mapped onto a corresponding system in which nearest-neighbor pairs of spins interact with energy $J = \infty$ if they are connected by a bond, or $J = 0$ if they are not connected by a bond. This mapping, which connects the CK theory to the Kastelyn–Fortuin[5] framework, suggests that the correlations in the Ising model are carried only by clusters of spins connected by bonds. Consequently, the Ising system can be separated into a collection of independent clusters, or "eigenclusters" of all sizes, which carry the correlations but do not interact with each other. Based on this idea, Swendsen and Wang[6] later developed a fast dynamical Monte Carlo algorithm for equilibrating the Ising model in which these eigenclusters are flipped with probability 1/2, allowing the system to take large steps in phase space directly to the equilibrium spin configuration, which drastically reduces the critical slowing down observed near T_c. It is straightforward to extend the CK formalism to an antiferromagnet. The interaction is satisfied if the nearest neighbor spins are anti-parallel and bonds are placed between these spins with probability p_b.

The identification of independent, correlated clusters of particles or spins in frustrated systems such as spin glasses and glass-forming liquids and polymers, has thus far remained elusive. We describe here an attempt to identify such clusters in the Ising spin glass model. The $\pm J$ Ising spin glass differs from the Ising model in that ferromagnetic and antiferromagnetic interactions are quenched randomly to the edges of the lattice. These competing interactions give rise to frustration when all the spins try to satisfy all the interactions simultaneously. The Hamiltonian for the Ising spin glass is:

$$-H = J \sum_{\langle ij \rangle} \epsilon_{ij} S_i S_j \,, \tag{5}$$

where the signs of the nearest neighbor interactions $\epsilon_{ij} = \pm 1$ are randomly distributed on the edges of a d-dimensional lattice. A loop (a closed path of edges) is considered frustrated if the spins in the loop cannot satisfy all the interactions (i.e., such that $\alpha_{ij} \equiv \epsilon_{ij} S_i S_j = 1$ for all nearest neighbor pairs in the loop). Consequently, a loop is said to be frustrated if the product of the signs of the interactions along the loop is negative, $\prod_{il}^{j} \alpha_{il} = -1$.

The Ising spin glass has a second-order thermodynamic transition at T_{sg} with exponents that differ from those of the Ising universality class. As in the Ising model, the transition is known to be characterized by a diverging correlation length (which in the spin glass is associated with the square of the spin-spin correlation function) and is accompanied by a strong divergence in the nonlinear susceptibility. However, the spin glass exhibits a breaking of ergodicity at T_{sg} that is much more severe than that in the Ising model at T_c, and displays an apparent ergodicity-breaking with complex dynamical behavior characterized by stretched exponential relaxation of autocorrelation functions well before the transition is reached.

The standard CK definition of clusters in the Ising model can be extended to frustrated systems. Again, clusters are defined as nearest-neighbor spins satisfying the interaction and connected by fictitious bonds with probability $p_b = 1 - \exp(-2J/k_B T)$. However, because of the two types of interactions in the spin glass, there are two ways for a pair of spins ij to belong to the same CK cluster — parallel and antiparallel to each other. Thus the probability p_{ij} of two spins i and j belonging to the same CK cluster can be written as:

$$p_{ij} = p_{ij}^{+} + p_{ij}^{-} \,, \tag{6}$$

where p_{ij}^{+} (p_{ij}^{-}) is the probability that: (1) spins i and j are connected by at least one path of bonds; and (2) the product η_{ij} over all the signs ϵ_{mn} along the path connecting i and j is $+1$ (-1). Thus $\eta_{ij} = 1(-1)$ implies that ij are parallel (antiparallel). Just as in the Ising case, the length ξ_p associated with the pair connectedness function $\overline{p_{ij}}$ diverges at the percolation temperature T_p (the bar represents the average over all possible interaction configurations ϵ_{ij}). However, this temperature does *not* coincide with the thermodynamic transition temperature in the spin glass, because the spin-spin correlation function $g_{ij} \equiv < S_i S_j >$ is no longer equal to p_{ij}, but instead is given by the *difference* between the two pair-connectedness functions[7]:

$$g_{ij} = p_{ij}^{+} - p_{ij}^{-} \,. \tag{7}$$

Because of the frustration caused by the competing interactions, the correlations are not carried by the CK clusters as they are in the Ising model. Note that for a given configuration, all the connected paths between i and j, i.e., all possible η_{ij}, will either be 1 or -1. At low temperatures most interactions which are satisfied will have a CK bond, hence sites i

and j will almost always be connected either with parallel or antiparallel paths. A revised definition of connectivity must be invoked to identify the spin glass eigenclusters.

The length ξ associated with $\overline{g_{ij}^2}$, diverges at the transition temperature T_{sg}, which is lower than T_p, due to the interference of paths with different phases as described above. Thus the effect of the frustration can be interpreted as a dilution of the effective correlations, pushing the transition temperature to a lower value than in the unfrustrated system. (In the ferromagnetic Ising model, two spins cannot be antiparallel and satisfy the interaction, and thus $p_{ij}^- = 0$.) To obtain the thermally-correlated eigenclusters in the spin glass, one must require that the pair correlation function be equal to the pair connectedness function for those clusters. One way to accomplish this in an approximate fashion is to dilute the CK clusters in such a way that bonds are retained with a probability reflecting the strength of the local correlation of that pair, which depends on the location of the pair on the lattice. Because of the disorder in the quenched interactions, some nearest-neighbor pairs of spins will be more correlated than others at a given temperature, unlike in the unfrustrated Ising model, where $< S_i S_j >$ for any nearest-neighbor ij pair is the same. Thus the dilution cannot be performed uniformly in frustrated systems as was done for the ferromagnetic system.

For simplicity, we can construct new clusters that carry most of the correlations by putting bonds with probability p_b between pairs of spins (1) satisfying the interactions, and (2) whose value of the correlation $\epsilon_{ij} < S_i S_j >$ is greater than or equal to some threshold g_{th}. We choose this threshold to coincide with the value of g_{ij} at the location of the maximum of the g_{ij} distribution. (This criterion reproduces the thermally-correlated CK clusters in the case of the Ising model, since in that case the g_{ij} distribution becomes a delta function in the thermodynamic limit for any temperature, and thus all pairs automatically satisfy the

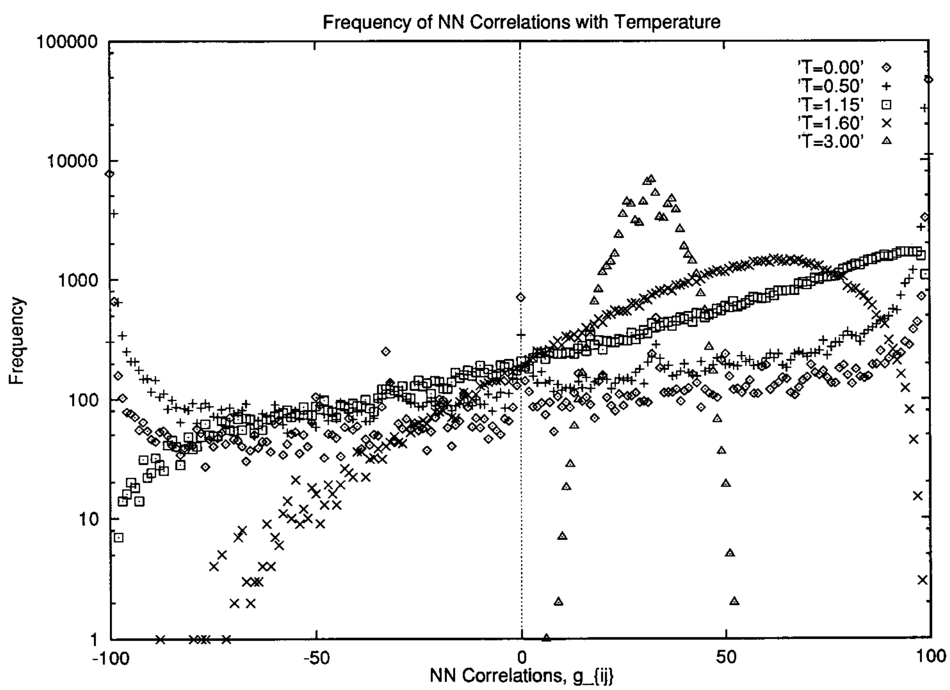

Fig. 1 The distribution of the nearest neighbor correlations for different temperatures. Note that at $T = 1.15$, the distribution spans the complete range.

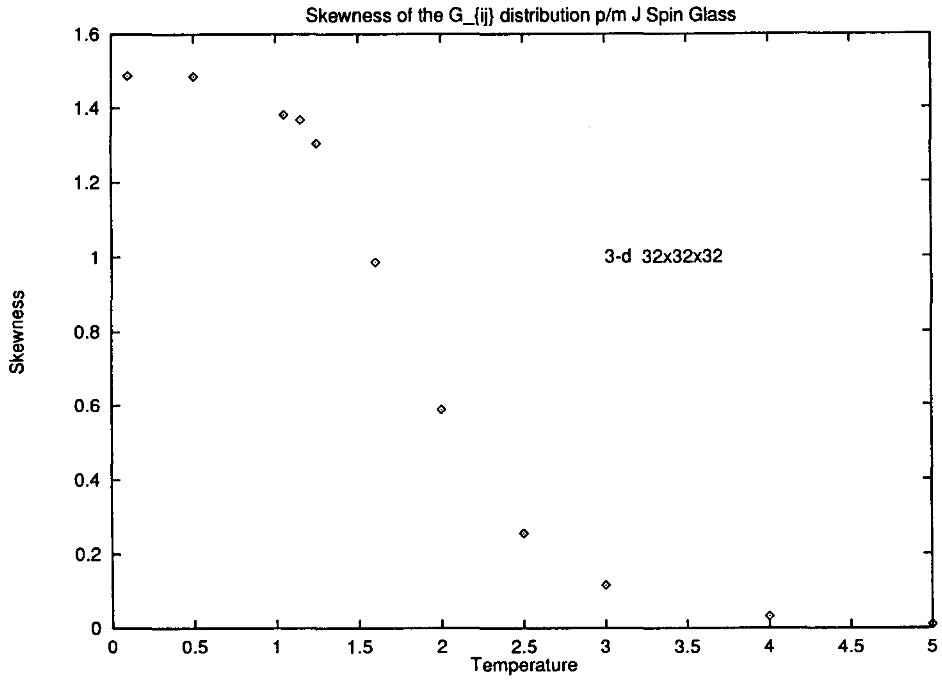

Fig. 2 The skewness of the distributions of Fig. 1 as a function of temperature.

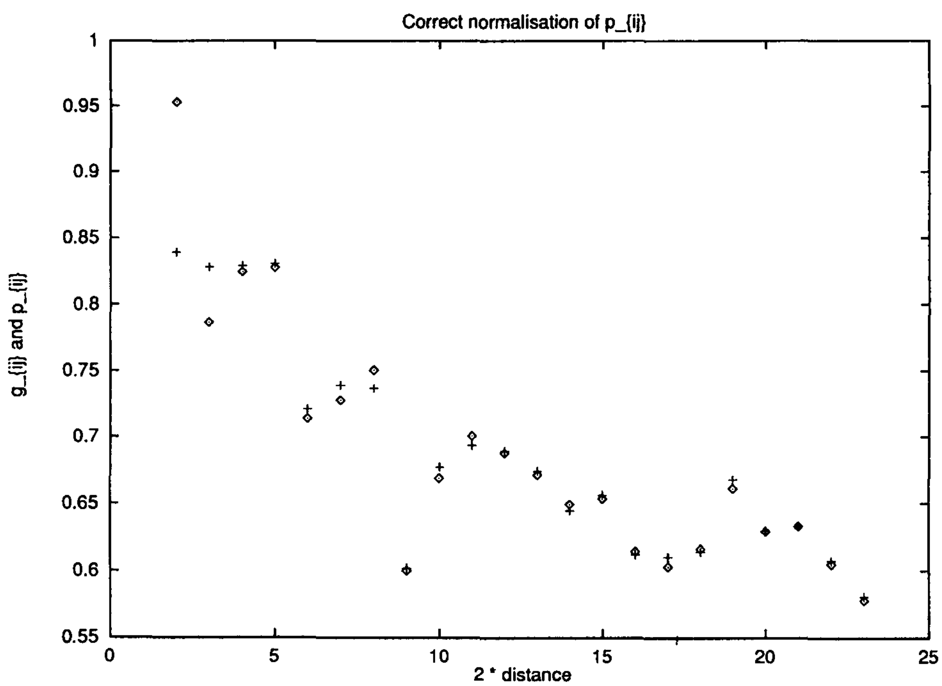

Fig. 3 The relation between g_{ij} and p_{ij}(difference) at $T = 1.15$, for a special site i and spherically averaged distance j.

second criterion.) Figure 1 shows the $\epsilon_{ij} g_{ij}$ distribution in the 3-d $\pm J$ Ising spin glass with system size 32^3, calculated for a number of temperatures above T_{sg}. We see that at the transition temperature, the distribution is sharply peaked near one, so that this criterion results in a subset of spins which are strongly correlated, or "quasifrozen".

The distribution of $\epsilon_{ij}g_{ij}$ values for the spin glass shown in Fig. 1 displays a number of interesting features. For example, at very high temperatures the distribution is not a delta function as in the Ising model, but rather a Gaussian whose width broadens with decreasing temperature. At a temperature $T \approx 4.0$, the distribution becomes asymmetric, and the asymmetry, or skewness, increases dramatically with decreasing temperature (see Figs. 2 and 3). This temperature at which the distribution becomes asymmetric is indistinguishable from the percolation temperature $T_p \approx 3.95$. Finally, at the spin glass temperature, the distribution drastically changes its shape, producing two sharply peaked maxima at the edges of the distribution. These maxima at $\epsilon_{ij}g_{ij}$ close to $+1$ and -1 represent pairs of spins that are almost permanently frozen ("quasifrozen") in satisfied or frustrated arrangements, respectively.

The search for the relevant clusters for the Ising spin glass should be considered as work in progress. We have not, as yet, found the appropriate eigencluster for the Ising spin glass but we feel that there is reason for optimism. The relevant clusters would be pivotal in a clearer insight into the nature of this complex system.

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