Towards a cluster description of the three-dimensional spin glass transition



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LETTER TO THE EDITOR

# Towards a cluster description of the three-dimensional spin glass transition

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**Abstract.** Numerically the three-dimensional transition in the Edwards–Anderson $\pm J$ spin glass agrees with the bond percolation threshold of the 'never' broken bonds.

In Edwards–Anderson spin glasses [1], each bond between nearest neighbours has randomly the energy $+J$ or $-J$, with equal probability, and the bonds connect spins $S_i = \pm 1$. In three dimensions, but not in two, a phase transition [2] is observed when the thermal energy $kT$ roughly equals the bond energy $J$. We call a bond between sites $i$ and $j$ 'broken' if in a given configuration $J_{ij}S_iS_j$ is negative ($= -1$); if this quantity is positive ($= 1$) we call the bond unbroken. It would be nice if the phase transition were connected to the percolation of unbroken bonds [3], as is the case for randomly dilute ferromagnets.

Such attempts at percolation descriptions for spin glasses are quite old [4], but a clear definition of how to define the percolating cluster is not easy. Even for pure ferromagnets this definition took a long time to develop; see chapter 7 of [3] for static and Alexandrowicz [5] for dynamic aspects. We get no agreement between the bond percolation threshold and the spin glass transition if we consider [6] unbroken bonds only with a probability $1 - \exp(-2|J|)$. This letter takes a step towards a suitable definition, leaving applications (like cluster flip algorithms [7]) to the future.

Liang [8] introduced the concept of observing empirically how often bonds are broken. In this spirit we observe the probability $w$ that during an observation time $t$ (measured in units of Monte Carlo steps per spin) a bond is found unbroken:

$$2w - 1 = \langle J_{ij}S_iS_j \rangle$$

for every neighbour pair. We then check for the bond percolation clusters formed by those bonds which had $w$ greater than some probability $W$, and by varying this probability $W$ we find its threshold value $W = p$ at which for the first time a bond percolation cluster spans the whole lattice. Then those bonds which are observed to be unbroken at least $pt$ times during $t$ sweeps through the lattice form an incipient infinite percolation cluster. (We check the bonds after every sweep.)

Figure 1 shows our results for this percolation threshold $p$ (in the form of $2p - 1$ which comes directly from summing up $J_{ij}S_iS_j$ over all time steps). The three-dimensional data approach the limit $p = 1$ at or slighly below $kT/J = 1.2$, close to the current estimates [9] of 1.18 to 1.34. Thus *at the spin glass phase transition, the 'never' broken bonds start to form an infinite cluster.*

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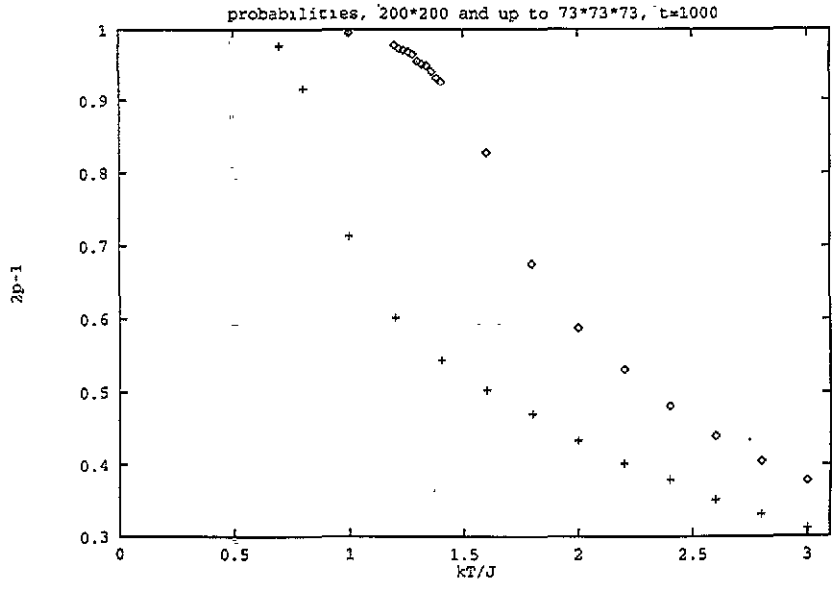


**Figure 1.** Percolation phase diagram in two dimensions. In the lower left part, an infinite network of seldomly broken bonds is formed. We observed ten consecutive intervals of length $t = 1000$, ignoring the first ones.

Unfortunately, this simple criterion cannot be exact since 'never' is a dangerous concept. If the observation time $t$ is long enough, a bond will always be broken at some time. For example, a spin surrounded by six ferromagnetic bonds and six parallel neighbours will flip to an antiparallel orientation with probability $\exp(-12J/kT) = 0.000\,05$ and thus break its bonds. Thus by increasing the observation time $t$ we should find the above thresholds to vary slightly, and this indeed is shown in figure 2 to be the case. A proper definition thus should use a very low but positive cut-off probability such that bonds broken less often than this cut-off are still regarded as unbroken. We have not found such a definition of 'rarely' broken bonds here, and thus our statement on the percolation of never-broken bonds is only approximative.

Figures 1 and 2 also show our two-dimensional results, giving an apparent phase transition near $kT/J = 0.7$. This temperature would be regarded as a phase transition point also from direct Monte Carlo simulations of short duration. Compared to three dimensions, however, our two-dimensional data seem to depend more strongly on observation time $t$.

Figure 3 shows histograms how often bonds are broken or unbroken. We see a maximum close to, but not exactly at, unit probability: during sweeps 9001 to 10 000 through the lattice, the largest number of bonds were broken three times and unbroken 997 times at $kT/J = 1.2$. For higher temperatures the histograms are more symmetric and stable in time.

The clusters formed by rarely broken bonds are not those of random percolation theory but strongly correlated due to the thermal interactions between the spins. Thus the number of bonds forming the incipient infinite cluster at the transition point $kT/J = 1.2$ is about 7.5 percent of the total number, as opposed to 24.9 percent at the random percolation threshold in this simple cubic lattice. Our number was found from 4 million sweeps through a $20 \times 20 \times 20$ lattice, showing little variation with time.

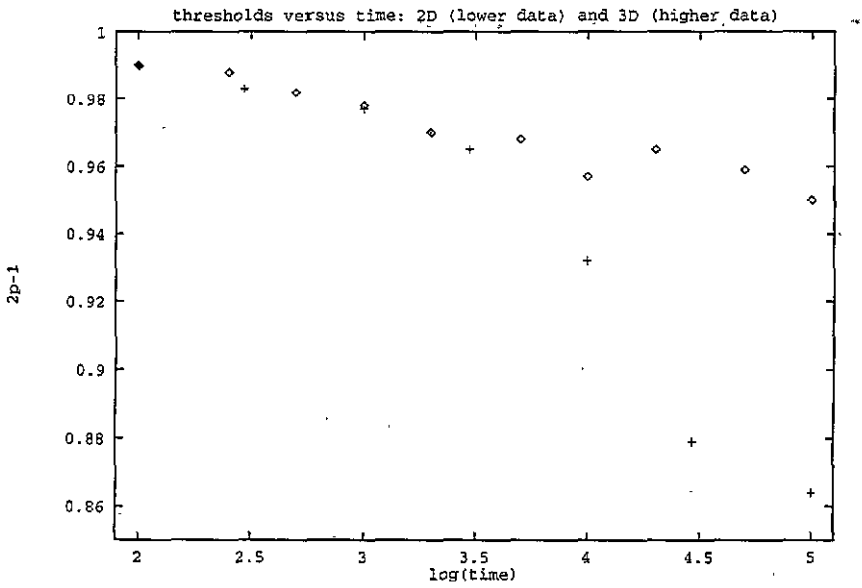


**Figure 2.** Percolation threshold versus decadic logarithm of observation time, for (typically) $200 \times 200$ (crosses, $kT/J = 0.7$) and $31 \times 31 \times 31$ (squares, $kT/J = 1.2$) lattices.

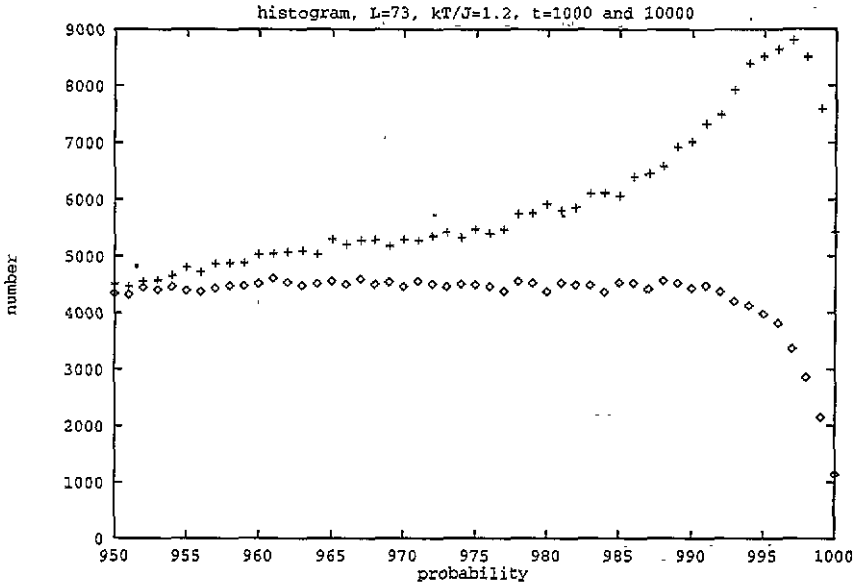


**Figure 3.** Histogram showing how many bonds had a given probability to be unbroken, during the interval from 1 to 1000 (squares) and from 9001 to 10 000 (crosses) sweeps through the $73 \times 73 \times 73$ lattice at $kT/J = 1.2$.

In summary, the rarely broken bonds start to form an infinite cluster of correlated bond percolations at the three-dimensional spin glass transition. This observation, however, is at best only one step towards a complete cluster description of spin glasses. After a clarification of the questions left open here, one should investigate the properties of these clusters and

their relationship to spin glass properties, the possibility of faster cluster-flip algorithms, and the transition between the cluster descriptions of spin glasses and ferromagnets.

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