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Metastable states in disordered ferromagnets

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Abstract. One-, two- and three-dimensional Ising spin-glass systems with Gaussian nearest-neighbour couplings, J_{ij}, are compared to their corresponding ferromagnetic systems in which the couplings are taken as $|J_{ij}|$. The local energy minima of systems consisting of not more than 16 spins were studied exactly. The larger systems were studied by a Monte Carlo method. Both systems have an exponentially growing number of minima. We analyse the energy and magnetisation distribution across these minima. In the ferromagnetic case a significant portion of the minima is only slightly magnetised. In the spin-glass case the absolute value of magnetisation, when averaged over the minima, shows a universal behaviour.

1. Introduction

The presence of many metastable states, i.e. local energy minima, is the essence of spin-glass physics. A common perception, however, is that disordered ferromagnets (DFM) are distinctively different from spin glasses (SG). For one thing, DFM are thought to be unfrustrated and, secondly, they are considered to possess only one energy minimum—the ground state. It is certainly true that the ground state of a DFM is very easy to specify since it simply corresponds to a complete spin alignment. With all of the couplings being positive there is certainly no frustration in this state: each exchange coupling multiplied by the spins it connects is positive.

In this paper we show, however, that the ground state of a DFM is but one of many local energy minima which are almost all frustrated. So the principal question asked in this paper is what really is the difference between a DFM and a SG if the absolute values of exchange couplings in both systems are identical. In the case of Ising spins, on which we focus here, the differences turn out to be more of quantity than of quality. This, in particular, suggests that the dynamics of the two systems should be very similar. This agrees with the prediction of Hertz (1983) and means that, for dynamical reasons, the DFM may not even get into the vicinity of its true ground state within experimental timescales.

The system we shall study is described by the Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} S_i S_j \tag{1}$$

where $S_i = \pm 1$. We shall mostly be interested in the Edwards-Anderson (1975) model of SG. In this model the exchange couplings J_{ij} are Gaussian random numbers of unit dispersion. In the corresponding DFM model the couplings are absolute values of the

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Gaussian numbers. A transition between such SG and DFM has recently been studied by Załuska-Kotur *et al* (1987) by the Migdal-Kadanoff method. The transition is driven by increasing the concentration of the negative bonds.

The case of J_{ij} being equal to -1 with probability x, and $+1$ otherwise, is very special due to the enormous degeneracies involved. The physics of this case at $x = 0.5$ (full frustration) and $x = 0$ is very different and it is not an object of the present studies.

2. Number of energy minima

A good starting point is to convince oneself that a DFM does have many local energy minima. The minima are defined here as states which are stable against single spin reversals. Figure 1 shows three plaquettes, or rings, with the exchange couplings arranged so that the weaker couplings alternate with the stronger ones. In figure 1(a) all of the J_{ij} are positive. This is a prototype DFM. By scanning through its 16 possible states we easily conclude that two of these (plus their inverted images) are such that turning any individual spin upside-down requires energy. These two stable energy minima are shown in figure 1 together with the corresponding energy and magnetisation per spin, M. The true ground state is fully aligned. The higher minimum is not magnetised and it gives rise to two frustrated bonds. These are the two weaker bonds.

Figures 1(b) and (c) show prototype SG in which two non-trivial energy minima also appear. In the case of (b) one bond is negative. Here, both minima frustrate a single bond each. In the case of (c) two bonds are negative (note that $\langle J \rangle = 0$) but the

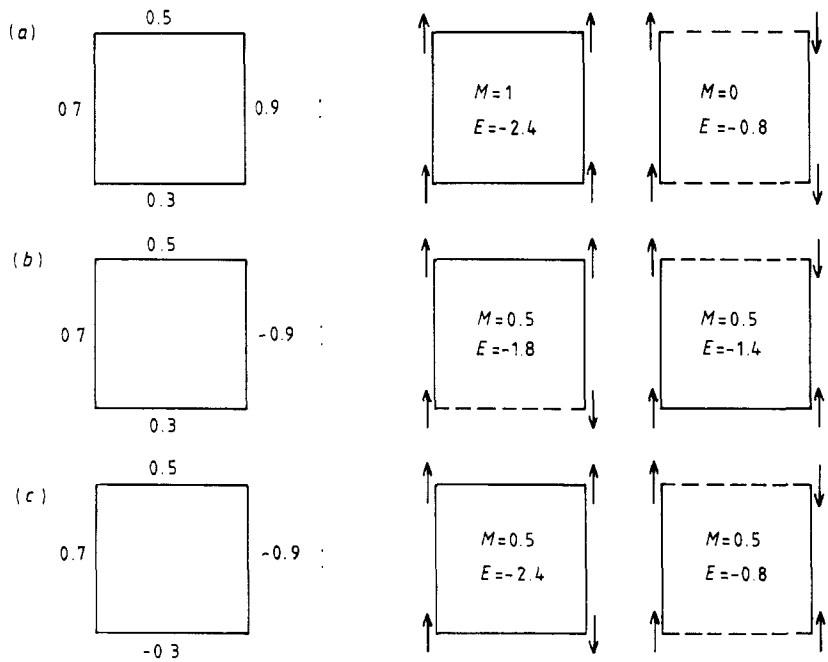

Figure 1. A ring of four spins with the exchange couplings as indicated. In (a) all the couplings are positive, in (b) one is negative, in (c) two are negative. The corresponding local energy minima are shown to the right. A broken line signifies a frustrated bond.

true ground state is not frustrated at all. It is the excited minimum in which two bonds are frustrated. In none of these states does M disappear.

A ring of four spins is nothing else but a small one-dimensional system with periodic boundary conditions. An interesting question to ask is how does the average number of stable energy minima $\langle n \rangle$, grow with the number, N, of spins. In order to answer this question we have performed an exact numerical analysis of $N \leqslant 16$ chains with periodic boundary conditions. For any given sample we have scanned through its spin states and selected all those which are stable against single spin reversals. Only non-trivial energy minima have been counted, i.e. an inverted minimum has not been considered as a new minimum. For $N = 6$ and 8 we have studied 800 samples, both in the DFM and SG case. For $N = 10$, 12, 14 and 16, we have searched 600 different samples for minima.

Even though the eigenenergies of each DFM sample differ from those of the corresponding SG system, their number of minima, and hence $\langle n \rangle$, has been found to be precisely the same. This common dependence of $\langle n \rangle$ on N is shown in figure 2. The statistical scatter is less than the size of the data points. The increase in $\langle n \rangle$ is exponential:

$$\langle n \rangle = n_0 \, e^{N/\alpha} \tag{2}$$

where $n_0 = 0.4993$ and $\alpha = 4.1398$. Since $e^{1/\alpha} = 4/\pi$ this result agrees exactly with the $(4/\pi)^N$ law derived by Derrida and Gardner (1986) under assumptions of (a) symmetric probability distribution for J_{ij} (not satisfied by DFM) and (b) large systems. This law, then, is more general.

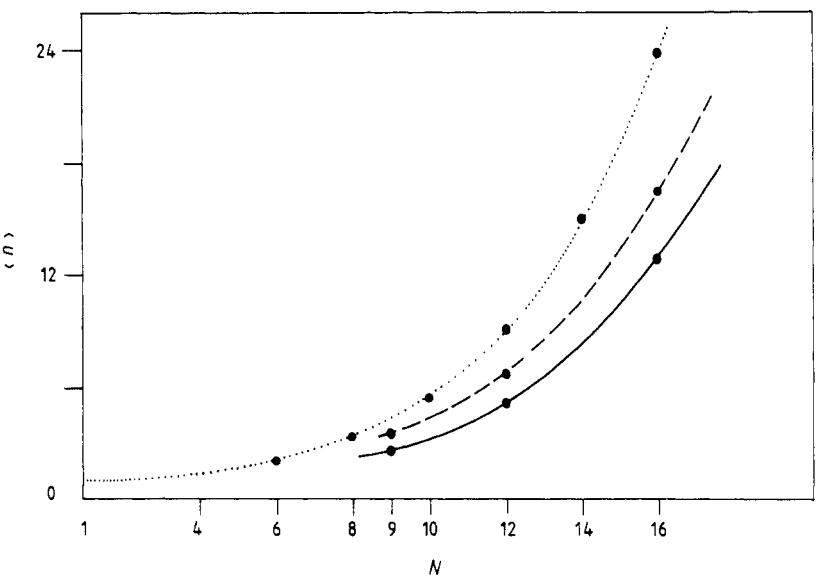

Figure 2. Average number of non-trivial local energy minima plotted against the number of spins. The full curve corresponds to a two-dimensional SG with the Gaussian couplings. The broken curve is for the two-dimensional DFM. The dotted curve is for both the SG and DFM one-dimensional systems. All of the curves are fits to equation (2) with the parameters as described in the text.

In the case of two-dimensional systems, DFM and SG begin to differ, as also shown in figure 2. The sizes considered are 3×3 (i.e. $N=9$), 3×4 and 4×4 and the numbers of samples are 800, 800 and 600 respectively. Again $\langle n\rangle$ grows exponentially in both models. In the case of SG the growth can be described by equation (2) in which $n_0=0.51$ and $\alpha=4.61$. In the case of DFM the growth is slightly weaker: $n_0=0.37$ and $\alpha=4.50$. Note that α is somewhat larger in two-dimensional systems than in one-dimensional systems. The reason is that in two-dimensional systems there are more conditions to be satisfied for a state to become a stable energy minimum. It follows that in three-dimensional systems $\langle n\rangle$ should grow with N still weaker. Unfortunately studying reasonably sized three-dimensional systems was beyond our reach. Note that $\langle n\rangle$ as a function of the linear size, $L=N^{1/d}$, of the system should grow stronger and stronger with the dimensionality. This is because the number of states grows extremely fast on increasing d for a given L.

Another way to characterise the number of the energy minima is to specify $\langle \ln n\rangle = a+N/b$. This quantity, as opposed to $\langle n\rangle$, is an extensive one. For the one-dimensional systems we obtain $a=-0.6858$ and $b=4.3234$. For the two-dimensional systems we obtain $a=-1.1422$, $b=4.4307$ in the DFM case and $a=0.7922$, $b=4.5413$ in the SG case. The conclusions remain qualitatively the same.

3. Density of metastable states

A next question to ask is what the energy distribution of the local energy minima is. The distribution of such states will be denoted by $n(\varepsilon)$, where $\varepsilon=E/N$ measures the energy per spin. Small systems can be studied exactly. The bigger ones, however, are amenable to Monte Carlo methods and then only the 'most important' states are seen of all the relevant phase space. Our numerical procedure was as follows. We took at least 200 samples and in each a random spin configuration was selected. Then we set the temperature T to be equal to 2.0. After five Monte Carlo steps per spin T was reduced to 1.5. After the next five Monte Carlo steps per spin, T became 1.0, then similarly 0.5 and finally 0. At that stage the system underwent an energy minimisation until no further decrease in energy was possible. The procedure was repeated at least 100 times for each sample. Changing five Monte Carlo steps per spin into 100 was checked and found not to affect the results in any significant manner.

Figure 3 shows results obtained for one-dimensional systems. The systems with $N=8$ and 16 were studied exactly and with $N=100$ by the Monte Carlo method. In each case the histograms for SG and DFM are almost the same and are both symmetric. The width of the distribution shrinks with N logarithmically.

Figure 4 shows exact results on $n(\varepsilon)$ for the 4×4 systems and Monte Carlo results for the 15×15 systems. The metastable states of a SG are distributed symmetrically whereas those of a DFM form a low-energy tail, indicating less frustration.

Similar features are seen in figure 5 showing Monte Carlo results obtained on $3\times3\times3$ and $6\times6\times6$ systems. As opposed to one- and two-dimensional data, the distribution of energy minima in a DFM is significantly broader than in a corresponding SG and the low-energy tail is much more pronounced.

Both in two- and three-dimensional systems the distributions corresponding to DFM have their centres of mass, as marked by arrows, shifted towards lower energies compared to the SG distributions (in the case of 4×4 systems the shift is very small).

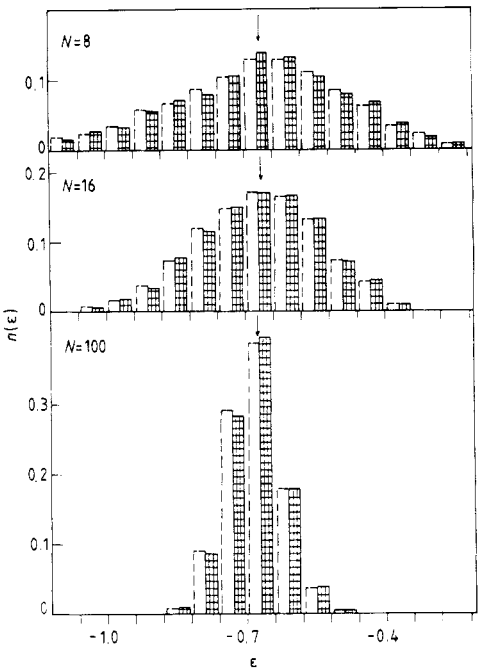

Figure 3. The density of local energy minima plotted against energy per spin in the one-dimensional systems. The full lines refer to the DFM and the broken lines to the SG. The vertical lines comprise a histogram corresponding to exact results obtained for the $N = 16$ systems. The data have been obtained for the $N = 100$ systems by the Monte Carlo method. The energy per spin intervals are equal to 0.06. The arrows indicate an average ε.

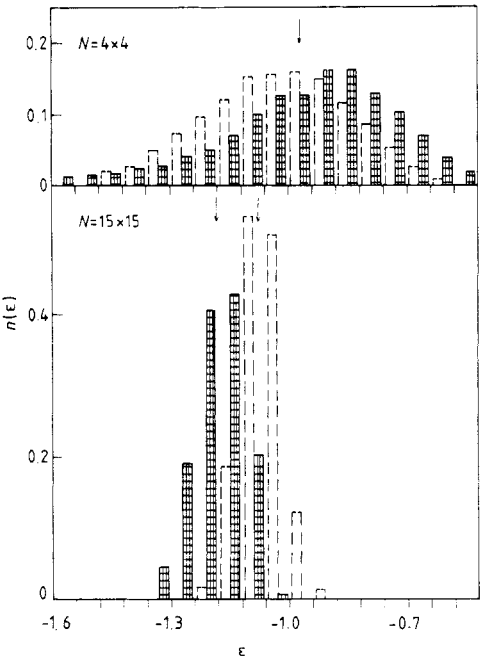

Figure 4. Same as figure 3 but for two-dimensional systems. The exact results (vertical lines) are for $N = 4 \times 4$ and Monte Carlo results for $N = 15 \times 15$. In the 15×15 case the full arrow indicates $\langle \varepsilon \rangle$ in the DFM case and a broken one in the SG case. In the 4×4 case the two arrows coincide.

The average energy per spin presumably saturates at a constant value on increasing N. In the one-dimensional case $\langle \varepsilon \rangle$ is almost the same for each N studied.

So far we have been concerned with the average distributions of the metastable states. Such distributions, or more precisely distributions of the energy barriers, may be of interest when studying spectra of relaxation times. The low-temperature thermodynamics, however, is determined by the average logarithm of the density of metastable states. This 'residual entropy' has been studied by Bray and Moore (1981) and Ettelaie and Moore (1985). The latter paper contains a detailed discussion of the one-dimensional SG.

Our Monte Carlo results for $\langle \ln n(\varepsilon) \rangle$ are shown in figure 6. In order to make a better comparison between DFM and SG, a distribution of n in each sample is first normalised to unity by dividing it by the total number of minima found in that sample. The states are allocated to bins according to their energy per spin and the bin width is equal to 0.1. Logarithms of the occupation numbers obtained in this manner are then averaged over 200 samples. From figure 6 we can see that, both in the two- and three-dimensional cases, the distribution of $\ln n(\varepsilon)$ is much broader for the DFM systems than for the SG ones. Furthermore the states from the low-energy tail carry much more thermodynamic weight in the DFM than in the SG.

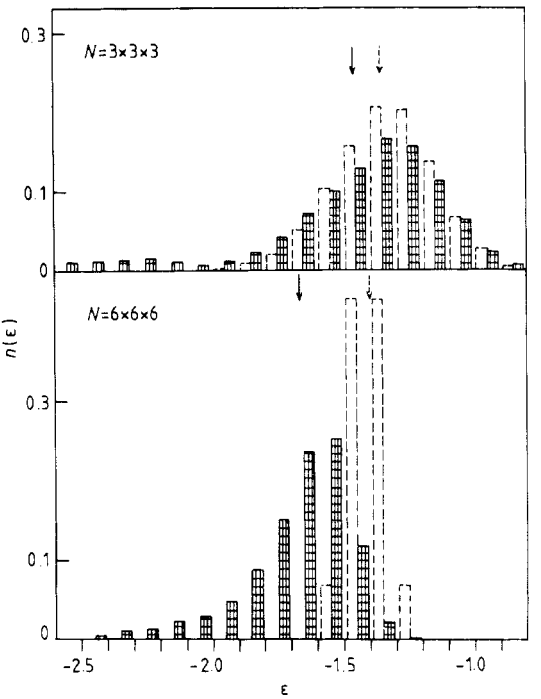

Figure 5. The density of metastable states plotted against the energy per spin in the three-dimensional systems. The full lines refer to the DFM case and the broken ones to the SG. These are Monte Carlo data on $3\times3\times3$ and $6\times6\times6$ systems as indicated in the figure. The energy per spin intervals are equal to 0.1. The full (broken) arrow indicates $\langle\varepsilon\rangle$ in the DFM (SG) case.

4. Magnetisation

One intuitively expects DFM to be more magnetised than the corresponding SG. We find that this is indeed the case. However, the bulk of the ferromagnetic metastable states is magnetised very little.

Consider the one-dimensional data first. These are shown in figure 7. The data for $N = 16$ are exact and for $N = 100$ they come from the Monte Carlo calculation. The $N = 16$ systems allow for nine different values of $|M|$ but there is no metastable state with $|M| = \frac{14}{16} = 0.875$. In the DFM case there is always a fully magnetised minimum in each sample. The most probable state, both in DFM and SG, corresponds to $M = \frac{2}{16} = 0.125$. However the DFM magnetisations are spread more evenly across the allowed values.

For $N = 100$, $|M|$ occurs most frequently between 0 and 0.1. The fully magnetised state has never been reached. The average magnetisation is reduced for both SG and DFM. Still, however, DFM states are more magnetised.

Derrida and Gardner (1986) show that in the one-dimensional SG case there should be no metastable states above $|M| = 0.446\,042$. Our Monte Carlo data do not contradict this statement. However, our results for $N = 16$ do yield several states above the limit set by Derrida and Gardner. Perhaps the constraint on $|M|$ holds only in the thermodynamic limit.

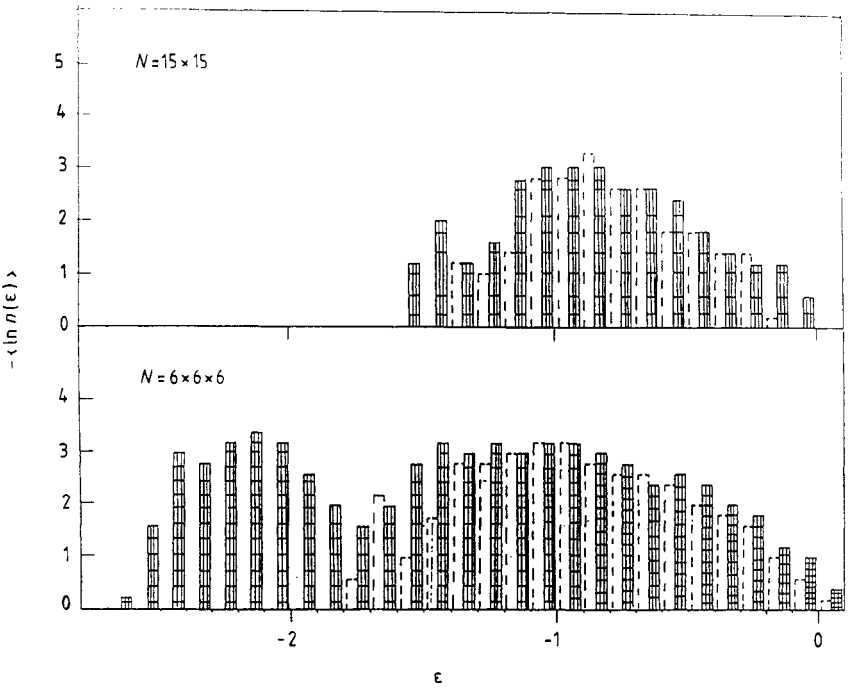

Figure 6. Distributions of $-\ln n(\varepsilon)$ where $n(\varepsilon)$ is the number of minima having energies per spin between $\varepsilon - 0.05$ and $\varepsilon + 0.05$, for $N = 15 \times 15$ and $N = 6 \times 6 \times 6$ systems. $n(\varepsilon)$ is normalised to unity in each sample. The full lines correspond to DFM and the broken ones to SG.

Figure 8 shows $|M|$ as found for the two-dimensional systems. The 4×4 systems were studied exactly and the 15×15 systems by the Monte Carlo method. The magnetisation behaves very similarly to the one-dimensional case. Even the average $|M|$ almost coincides at the two common values of $N = 16$, both for DFM and SG.

Figure 9 corresponds to the three-dimensional systems. Both sizes, $3 \times 3 \times 3$ and $6 \times 6 \times 6$, were studied by the Monte Carlo method. The minima of the three-dimensional DFM samples are significantly more magnetised than those of the SG samples. They are more uniformly spread out and the vicinity of $|M| = 1$ is no longer avoided. Nevertheless the minima of low $|M|$ are most probable. As expected, the SG minima are increasingly less magnetised when N is enlarged.

Figure 10 compares $|M|$ averaged over all metastable states for various sizes and dimensionalities regardless of the method of calculation employed. It is interesting to notice that $\langle |M| \rangle$ of SG systems decreases logarithmically with N and seems to depend exclusively on N. The one-, two- and three-dimensional data points lie essentially on the same curve. Furthermore, the distribution of the exchange couplings appears not to matter either. We have investigated exactly the $N = 10$ and $N = 16$ one-dimensional systems with a rectangular distribution of J_{ij} and found that the results also fit the curve obtained for the Gaussian couplings.

The DFM systems are much more sensitive to the geometry and to the details of the distribution of the couplings. The one-dimensional systems yield a line above the SG one and also suggest a $1/\ln N$ decay of $\langle |M| \rangle$. The one-dimensional systems with the rectangular distribution of J_{ij} (not shown in the figure) give rise to a still different curve.

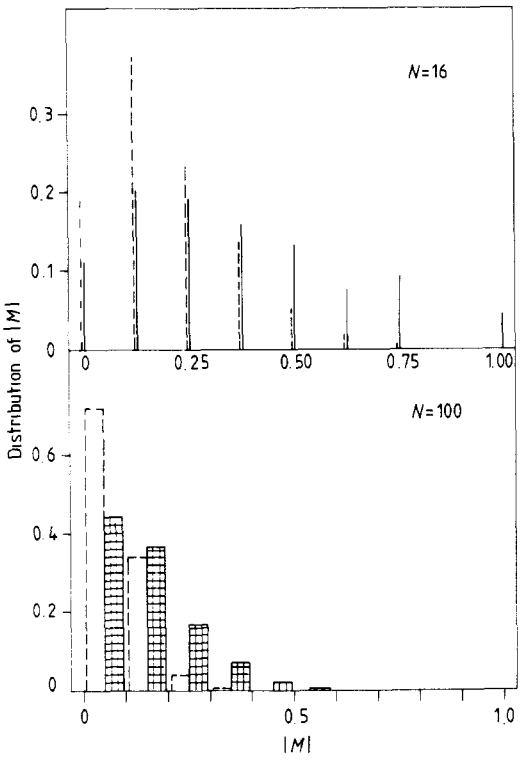

Figure 7. Distribution of the absolute value of magnetisation per spin across the local energy minima of one-dimensional systems. The full lines correspond to DFM and the broken ones to SG. The figure shows exact results for $N = 16$ systems and Monte Carlo results for $N = 100$.

The statistics of 20 000 minima is insufficient to determine trends of behaviour of $\langle |M| \rangle$ for two- and three-dimensional DFM with certainty. Large widths in the distribution of $|M|$ make it difficult to determine the precise average value of $|M|$—the width is of the order of the average. It seems that the two- and three-dimensional DFM yield two separate curves above the one-dimensional results. The decay of $\langle |M| \rangle$ in three-dimensional samples appears to be very slow. In fact, a possibility of saturation at a constant value cannot be ruled out if a sufficient size is reached.

Our main conclusion is that disordered Ising ferromagnets are, in many respects, very much like spin glasses: they have exponentially growing numbers of local energy minima. A significant portion of these minima are only weakly magnetised. The three-dimensional systems distinguish most tangibly between SG and DFM in quantitative measures. The one-dimensional DFM and SG systems with the same $|J_{ij}|$ have identical distributions of the energy minima and they differ merely by the properties of the magnetisation.

The lower critical dimensionality of DFM Ising systems, however, is different from that of corresponding spin glasses and remains equal to 1, i.e. as in the case of uniform couplings. One can be convinced of this by testing the sensitivity of the system to changes in the boundary conditions (see, e.g., Binder and Young 1986, Banavar and Cieplak 1982). Unlike the spin glasses, the lowest energy of DFM is always realised with the periodic boundary conditions and a twist in 'wall potentials' remains localised

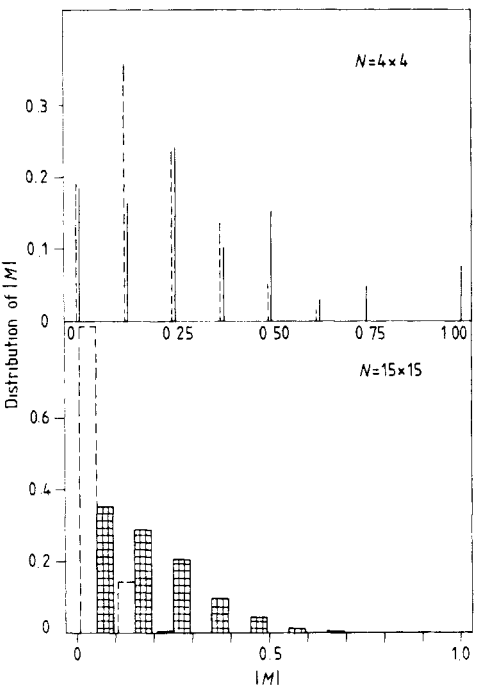

Figure 8. Same as figure 7 but for two-dimensional systems, showing exact results for $N = 4 \times 4$ systems and Monte Carlo results for 15×15 systems.

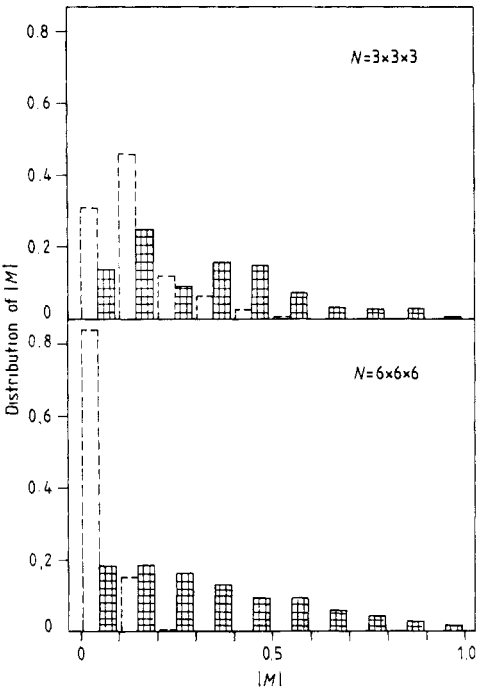

Figure 9. Same as figure 7 but for three-dimensional systems, showing the exact results for $N = 3 \times 3 \times 3$ and $N = 6 \times 6 \times 6$ systems.

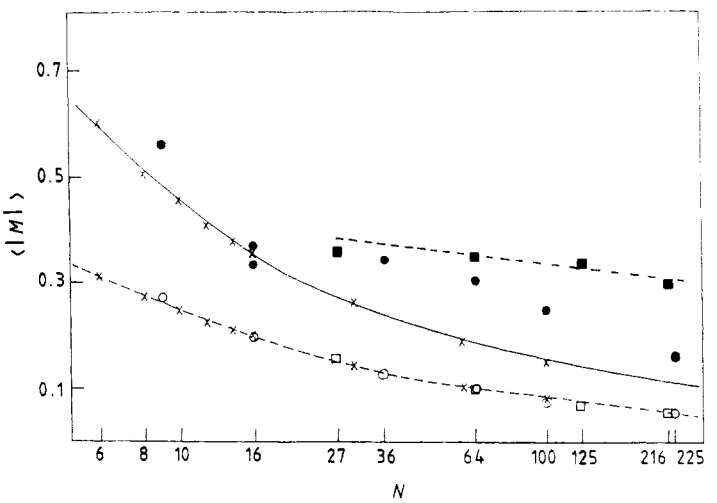

Figure 10. Average absolute value of magnetisation plotted against $\ln N$ for one-dimensional samples (×, joined by the full curve for DFM data and by the lower broken curve for SG data), for two-dimensional samples (●, DFM; ○, SG) and for three-dimensional samples (■, DFM; □, SG). There are two data points corresponding to the two-dimensional 4×4 DFM; the upper point was obtained by the Monte Carlo procedure and the lower one through the exact enumeration of states. The upper broken line organises the three-dimensional DFM points.

on a weakest bond. The Heisenberg DFM also seem to have their lower critical dimensionality not modified by the disorder (Banavar *et al* 1982). In this case this dimensionality is equal to 2.

It would be interesting to compare isotropic and anisotropic Heisenberg ferromagnetic systems to their corresponding spin glasses. Furthermore, it would be interesting to find out whether the universal behaviour of $\langle |M| \rangle$ found in the SG Ising systems is still present in the Heisenberg spin glasses.

Acknowledgments

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