LETTER TO THE EDITOR

Susceptibilities of spin glass models: a Monte Carlo study

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Abstract. The Monte Carlo method has been used to study the behaviour of Ising model spin glasses. Both the double delta function and Gaussian distributions of interaction strengths have been considered. No evidence for cusp-like behaviour is obtained, but the susceptibilities appear to diverge at low temperature.

In a recent Letter (Rapaport 1977, hereafter to be referred to as I) we described the results of a study of an Ising model spin glass using high-temperature series methods. The model is defined by the Hamiltonian

\[ H = - \sum_{NN} J_{ij} S_i S_j - H \sum_i S_i \]  

and the random nearest-neighbour interactions \( J_{ij} \) are subject to the double delta function (DDF) distribution

\[ P(J') = p \delta(J' - J) + (1 - p) \delta(J' + J) \quad 0 \leq p \leq 1. \]  

Analysis of the zero-field susceptibility series for the body-centred cubic lattice indicated a ferromagnetic transition for a range of values of \( p \) near unity with a transition temperature \( T(p) \) which drops rapidly with decreasing \( p \). The behaviour of \( T_c(p) \) was shown to be very similar to that of the corresponding annealed system (Kasai and Syozi 1973). However, in the annealed case \( T_c(p) \) actually drops to zero, and there is a range of \( p \) values for which no transition occurs. The series analysis was unable to determine whether the same is true for the random system, or whether some entirely different kind of behaviour (e.g. a cusp-like transition to a spin glass phase) appears at intermediate \( p \).

The originally proposed spin glass models (Edwards and Anderson 1975, Sherrington and Kirkpatrick 1975), involve systems whose interaction strengths are random and Gaussian distributed:

\[ P(J') \propto \exp \left[ -(J' - J_0)^2 / 2J_0^2 \right] \]  

Mean-field analysis predicts cusps in both the susceptibility (\( \chi \)) and the specific heat (\( C \)) at \( H = 0 \). The results of Monte Carlo simulations for the case \( J_0 = 0 \) (Binder and Schröder 1976, Binder and Stauffer 1976) have been used to support the claim that for \( H = 0 \) there is a cusp in \( \chi \), but only a rounded peak in \( C \).
We have undertaken Monte Carlo studies of the DDF system in both two and three dimensions, and of the Gaussian system—for various $J_0$, including a repeat of $J_0 = 0$—in three dimensions. In this Letter we discuss the salient features of the results; a more detailed analysis will appear later.

The simulations were made using a simple quadratic lattice of size $61 \times 60$ in $d = 2$ dimensions, and a $17 \times 17 \times 18$ simple cubic lattice for $d = 3$. Toroidal periodic boundary conditions were imposed. The interaction strengths were chosen randomly according to the distributions (2) or (3); in the latter case the continuous distribution was replaced by a histogram of discrete values in order to improve computational efficiency. Several different types of initial spin configuration were employed—the ferromagnetically ordered and random states, and the final state from a previous run at a higher temperature. Each run involved 2400 passes through the entire lattice, attempting to flip each spin in succession according to a well-known procedure (e.g. Yang 1963). In order to permit the system to reach its equilibrium state the first 800 passes through the lattice were excluded from the final estimates. Runs were made at various temperature values $(T)$, and concentrations $(p)$ for the DDF model, or locations of the distribution midpoint $(J)$, in the case of the Gaussian. More than one run was made for each point; near features of interest (see below) as many as ten runs were made. Different starting configurations, interaction distributions and random number sequences were used for the various runs. The quantities measured were the zero-field internal energy and magnetisation, and their fluctuations $\Delta C$ and $\Delta \chi$.

The susceptibility results for the three systems are shown in figures 1–3. The specific heat and an expanded plot of $\chi$ for the $J_0 = 0$ Gaussian appear in figure 4. The results plotted are the averages over all the runs, and no data smoothing has been performed. For convenience (and with no loss of generality) we have assumed $J = 1$ in the DDF distribution, and a unit width Gaussian $(J_w = 1)$.

Two features of the results stand out strongly—the apparent low-temperature divergence of $\chi$ in both DDF and Gaussian systems over a range of $p$ or $J_0$, and the absence of a well defined cusp at intermediate values of $p$, (e.g. $p = 0.5$) or small $J_0$ (e.g. $J_0 = 0$). The insets in figures 1–3 show how $\chi$ varies with $p$ or $J_0$ at the lowest
Figure 2. Susceptibility of the $d = 3$ DDF Ising system (see caption to figure 1).

Figure 3. Susceptibility of the $d = 3$ Gaussian distribution system for various $J_0$. The inset shows how $\chi$ varies with $J_0$ at low temperature.

Figure 4. Specific heat ($C$) and susceptibility ($\chi$) for the $J_0 = 0$ Gaussian case ($\chi$ is an expanded version of the curve in figure 3).
temperatures considered. There is no analogous growth in the specific heat at low temperature. In the following discussion we will examine the DDF and Gaussian results separately.

We first consider the $d = 2$ and 3 DDF behaviour. At $p = 1$ the results agree with the known properties of the pure Ising ferromagnet—there is a strong divergence in $\chi$ at the critical point $T_c$ (here truncated owing to the finite lattice size), and $\chi \to 0$ as $T \to 0$. For $p < 1$, the $\chi$ peak becomes less sharp and shifts to lower temperature, and the anomalous low-temperature increase in $\chi$ develops. It may be argued that the reason why $\chi$ appears to have a smoothly rounded maximum (instead of a cusp) at intermediate $p$ (e.g. $p = 0.5$ in figures 1 and 2) is that the ordinate scale is too compressed; however, even when $\chi$ is plotted using an expanded scale the peak resembles the one which appears in figure 4—the results show no evidence of a sharp cusp. The similar $T_c(p)$ behaviour of the annealed and random versions of the DDF model predicted by series analysis (I) suggests a possible interpretation of the Monte Carlo results. In the annealed system $\chi$ diverges the transition point $T_c(p)$ provided that $p_0 < p < 1$ ($p_0 = 0.05, 0.66$ for $d = 2, 3$). As $p \to p_0^+$, the annealed $T_c(p) \to 0$ (see figure 1 of I), and in the range $1 - p_0 < p < p_0$ there is no transition. The Monte Carlo estimates of the temperatures $T_{\text{max}}(p)$ at which the $\chi$ maxima occur are close to the corresponding annealed $T_c(p)$ for $p$ near unity, but as $p \to p_0^-$ there is no indication that $T_{\text{max}}(p) \to 0$ as does the annealed $T_c(p)$. There is, however, the possibility that it is not $T_{\text{max}}(p)$ which corresponds to the transition temperature in the thermodynamic limit, but that the $\chi$ singularity is actually a narrow spike sitting on the low-temperature side of a smoothly rounded peak. Behaviour of this kind is known to occur in the specific heat of the annealed dilute-bond Ising model (Rapaport 1971, see also figure 1 of James (1971)). A singularity of this type is not necessarily amenable to study by Monte Carlo methods, but could still show up in the series analysis.

A further indication of the relevance of the annealed results when trying to understand the Monte Carlo data is that at the lowest temperature studied ($T = 0.1$) the maximum value of $\chi$ (now regarded as a function of $p$) is found to occur near $p = p_0$ (see the insets in figures 1 and 2). In other words, the apparent $T \to 0$ $\chi$ divergence is strongest near that value of $p(p_0)$ at which $T_c(p) \to 0$ in the annealed system. Taking into account both the series predictions (I) and the Monte Carlo results, we suggest that the transition temperature of the random model becomes zero at some value $p = p_s$ close to $p_0$, but that at lower values of $p$ the random and annealed systems exhibit different behaviour—in the former a $T = 0$ (or at least $T \ll 1$) transition (with divergent $\chi$) occurs when $p < p_s$, whereas in the latter it is known that there is no transition below $p_s$.

Domb (1976) recently pointed out that for $p = 0.5$ the high-temperature $\chi$ expansion contains only the leading order paramagnetic term, i.e. $\chi = 1/T$ for $d = 2, 3$. The Monte Carlo results fit this form provided $T \gg 2.6$, whereas $T_{\text{max}}(p = 0.5) \approx 1.5$ ($d = 2$) and 2.0 ($d = 3$); thus the paramagnetic behaviour, and also the validity of the high-temperature ‘expansion’ at $p = 0.5$, break down at a temperature significantly greater than $T_{\text{max}}$.

The Gaussian results for $J_0 = 0$ (figure 4) are similar to those of Binder and Stauffer (1976), with the exception of the low-temperature region which they apparently did not explore. However, whereas these authors claimed to detect a cusp in $\chi$, our results suggest that the maximum is smoothly rounded.

The inset in figure 3 shows that the $T \to 0$ increase in $\chi$ is strongest at $J_0 = 0$, and as $J_0$ increases this effect rapidly disappears. For sufficiently large $J_0$ ($J_0 = 1.5$) the finite width of the Gaussian ($J_0 = 1$) loses its importance and a ferromagnetic transition occurs at an expected $T_c(J_0) \approx J_0 T_c$ (Ising). Mean-field analysis (Sherrington and
Kirkpatrick 1975) correctly predicts that $T_c(J_0) \propto J_0$ for $J_0$ above a certain value, but below this value it predicts that $T_c(J_0)$ is constant and non-zero. The low-temperature divergence of $\chi$ revealed by the Monte Carlo results probably stems from the competing effects of the positive and negative short-range interactions present in the system (this is equally true for the DDF models); the mean-field treatment, with its introduction of infinite range interactions, cannot be expected to yield a correct picture since it ignores short-range effects.

Overall, the results indicate that some reassessment of the properties of these spin glass models is called for. It is by no means clear that an Ising system with short-range interactions of the type considered here is able to exist in a disordered, but stable, ‘spin glass’ phase at non-zero temperature. It also remains to be seen whether the apparent $T \to 0$ divergence of $\chi$ corresponds to a phase transition at $T = 0$ and, if so, whether this is a feature unique to models of this type, or whether it is a real effect which ought to be observable experimentally. (After this work was completed, the Monte Carlo study of the $d = 2$ DDF system by Sakata et al (1977) came to our attention. They claim to detect cusps in both $C$ and $\chi$, but closer examination of their data, which involves considerably fewer samples than used here, reveals that the presence of smoothly rounded peaks is equally likely.)

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References

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