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LETTER TO THE EDITOR

Residual magnetic entropy and metastable states of the Edwards–Anderson Ising spin glass

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Abstract. The residual magnetic entropy is calculated for the short-range Edwards–Anderson spin-glass model by the Monte Carlo method. For slow cooling, a finite value of the residual magnetic entropy is obtained, which depends only weakly on the cooling rate. A comparison with available information about the total density of states and the density of metastable states suggests that the residual magnetic entropy is determined by the density of metastable states at the residual energy of the spin glass at zero temperature.

Relaxation phenomena occurring on long time scales are a characteristic feature of spin glasses (for a recent review see Mydosh (1981)). Theoretically, such effects have been observed in numerical studies of the short-range Edwards–Anderson Ising model (for a recent review see Binder and Kinzel (1981)). These results, both theoretical and experimental, support the interpretation of the spin-glass transition as a non-equilibrium dynamic phenomenon (Morgenstern and Binder 1979) associated with the time scale τ_{obs} of experimental observation. For times $t < \tau_{obs}$ the system samples only a small part of the total phase space. Information regarding the fraction of the accessible phase space and the number of configurations or 'valleys' in which the system can settle may be obtained from the residual magnetic entropy. In this respect the spin-glass transition resembles the freezing process of ordinary glasses. The concept of the residual entropy of ordinary glasses has been discussed recently by Jäckle (1981). Owing to the small width of the transformation range and the metastability of the glass phase, the residual entropy obtained from specific heat measurements determines the number of metastable glass configurations with good accuracy. It is the main purpose of this letter to examine whether also in spin glasses the residual magnetic entropy, which determines the number of spin configurations populated at zero temperature, can be derived from thermodynamic measurements.

Irrespective of the uncertainty of its physical significance below T_f, an 'experimental entropy curve' $S_{exp}(T)$ can be calculated from a measured specific heat curve $C(T)$ using the thermodynamic formula

$$S_{exp}(T) = S(\infty) - \int_T^\infty \frac{dT'}{T'} C(T'). \tag{1}$$

For the Ising spin-$\frac{1}{2}$ model to be used in the Monte Carlo (MC) calculation, one has

$$S(\infty) = Nk_B \ln 2, \tag{2}$$

where N is the number of Ising spins. In the non-equilibrium region below T_f, the temperature T is defined as the temperature of a heat bath which determines the transition probabilities in the MC process. At zero magnetic field H the specific heat is given by the temperature derivative of the internal magnetic energy $U(T)$:

$$C(T) = \partial U/\partial T|_{H=0}. \tag{3}$$

By partial integration (1) is transformed into

$$S_{\text{exp}}(T) = S(\infty) - \int_0^{1/T} \mathrm{d}(1/T')[U(T') - U(T)] \tag{4}$$

which yields the entropy directly in terms of $U(T)$.

In thermodynamic or metastable equilibrium, the specific heat is related to the isothermal energy fluctuations by

$$C_{\Delta U}(T) = \overline{(\Delta U)^2}_T/(k_B T^2). \tag{5}$$

We shall compare MC data for the two different kinds of specific heat given by (3) and (5) and estimate the width of the transition region from observed differences between the two quantities. If this transition region has a relatively small width and contributes little to the entropy integral, the zero-temperature entropy $S_{\text{exp}}(0)$ obtained from (1) or (4) should be a good approximation to the residual entropy related to the number of different spin configurations occurring at absolute zero (Jäckle 1981). If, however, this width is large, the significance of the value $S_{\text{exp}}(0)$ can only be tested by comparison with a statistical-mechanical calculation of the residual entropy.

We have performed MC calculations for the two-dimensional Edwards–Anderson Ising spin glass of 60×60 spins on a square lattice with a Gaussian distribution of nearest-neighbour couplings. First we report the results of entropy calculations obtained from the internal magnetic energy $U(T)$ using (4). The energy curve $U(T)$ was calculated in temperature steps of 0.1 (in units of the root-mean-square fluctuation of the exchange coupling constants ΔJ). The spin system started in a random spin configuration at $T = 1.5$ and was cooled continuously from this temperature at different cooling rates. A value for $U(T)$ was obtained by averaging the total energy over the MC trajectory in the corresponding temperature interval. We calculated entropy curves $S_{\text{exp}}(T)$ for different values of the inverse cooling rate given by the length Δt (in MCS/spin) of the MC trajectory in each temperature interval. The maximum value of Δt was 1600 MCS/spin. Contrary to the entropy derived from the partition function summed over all spin space (Morgenstern and Binder 1980), the entropy curves have non-zero values $S_{\text{exp}}(0)$ for temperature zero. The dependence of these entropy values on cooling rate is shown in figure 1. From the variation of the results of different MC runs, the error is estimated to be about 10%. The data of figure 1 are compatible with the existence of a plateau with regard to the dependence of the values of $S_{\text{exp}}(0)$ on the cooling rate. If it is assumed that a plateau does exist, a probable value of the plateau is

$$S_{\text{exp}}(0)/k_B N = 0.04 \pm 0.01. \tag{6}$$

Estimating from this result the residual experimental magnetic entropy which is to be expected from measurements on a real spin glass, one has to bear in mind that a spin in the Edwards–Anderson model corresponds to some spin cluster in the dilute magnetic alloy (Binder 1977).

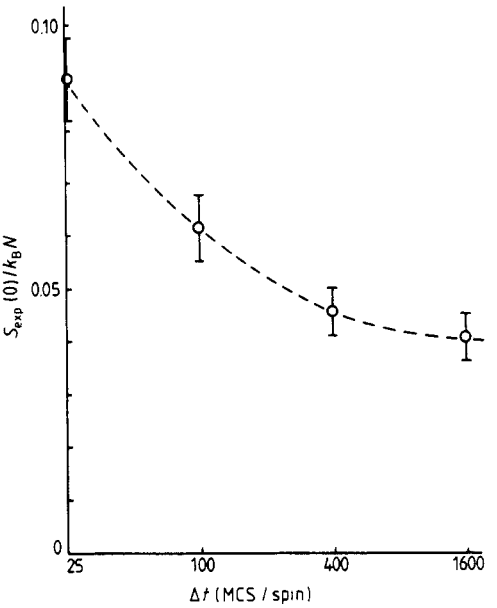

Figure 1. Dependence of the calculated 'residual experimental magnetic entropy' $S_{exp}(0)$ on the inverse cooling rate Δt. (The broken line is only a guide to the eye.)

Next we have tested the validity of the fluctuation formula (5) for the specific heat. To obtain $C_{\Delta U}(T)$, the energy fluctuations were sampled over a MC trajectory of 1000 MCS/spin at each temperature. Each trajectory started from a spin configuration which had been prepared before by slow cooling in (24000 MCS/spin) down to $T = 0.1$. Figure 2 shows the data for $C_{\Delta U}(T)$, averaged over ten different MC runs, together with the results for the energy derivative $C(T)$. Between $T = 1.0$ (which corresponds

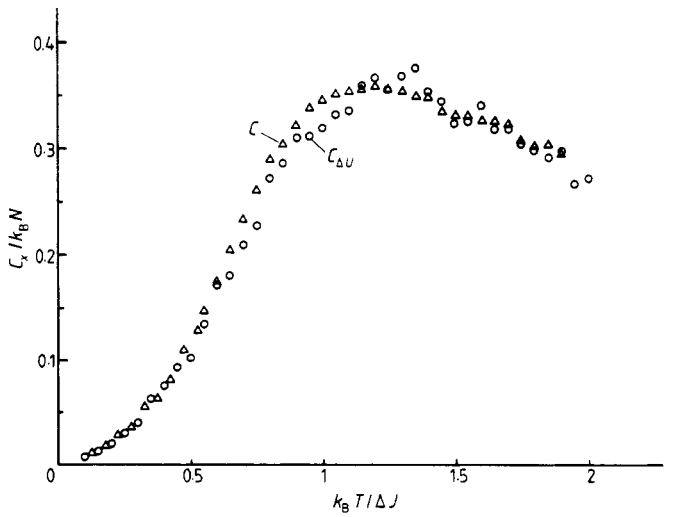

Figure 2. Specific heats derived from energy (C) and energy fluctuations ($C_{\Delta U}$) as a function of temperature.

to the freezing temperature T_f) and $T = 0.5$ the specific heat $C_{\Delta U}$ derived from the energy fluctuations is significantly lower than C. (The differences between $C_{\Delta U}$ and C at higher temperatures are statistically not significant.) As a consequence, the entropy $S_{exp}(T)$ calculated from $C_{\Delta U}(T)$ decreases more slowly with decreasing temperature than that derived from $C(T)$. The resulting difference between the zero-temperature limits of both types of entropy curves is

$$[(S_{exp}(0))_{\Delta U} - (S_{exp}(0))_U]/(k_B N) = 0.02. \tag{7}$$

We have checked whether this result depends on the particular choice of the initial spin configuration of our MC trajectories and found nearly identical results for a cooling process which started from a high-temperature spin configuration at the maximum temperature. Clearly, the discrepancy between the two results for the specific heat shown in figure 2 is a manifestation of the non-equilibrium behaviour of the spin-glass model on the time scale of our MC experiment. We conclude that on this time scale the spin-glass transition region, over which the spin-glass freezing occurs, is very broad and extends from T_f down to $T_f/2$. This finding is in marked contrast with the comparatively narrow width of the glass transition region of ordinary glasses.

To provide a basis for the discussion of the observed specific heat difference and the associated width of the transition region, an analysis of the spin-glass transition is now presented which extends the analysis of the ordinary glass transition in terms of configurations (Jäckle 1981). The continuous freezing process of the spin glass is idealised as a sequence of many discrete freezing steps at which the spin phase space is split successively. At a particular step at temperature T a single configuration with phase space Ω which is occupied at $T + \Delta T$ is split into several configurations i with phase space Ω_i. Only one of these configurations is occupied in a particular sample at $T - \Delta T$. It is assumed that at the higher temperature $T + \Delta T$ the occupation of the different parts of Ω corresponds to thermal equilibrium at this temperature, whereas the probability of finding the system in configuration i at $T - \Delta T$ is given by a quenched probability p_i^* which may be different from the equilibrium probability $p_i(T - \Delta T)$ that would exist at this temperature if no freezing occurred. Averaging over the different possibilities for trapping the system in different configurations i, the following formula for the difference between the two kinds of specific heat is obtained:

$$\begin{aligned} C(T) - C_{\Delta U}(T) &\equiv (2\Delta T)^{-1}[U(T+\Delta T) - U(T-\Delta T)] - \tfrac{1}{2}[C_{\Delta U}(T+\Delta T) + C_{\Delta U}(T-\Delta T)] \\ &= \sum_i \frac{p_i(T) - p_i^*}{2\Delta T} U_i(T) + O(\Delta T). \end{aligned} \tag{8}$$

Here, $U_i(T)$ is the internal energy of the system at temperature T averaged over the cell of phase space corresponding to configuration i. According to (8) the observed positive sign of the difference between C and $C_{\Delta U}$ implies a negative correlation between the deviation of the quenched probability p_i^* from the equilibrium probability $p_i(T)$ on one side and the average energy $U_i(T)$ of a configuration on the other. The configurations with higher energy tend to freeze out faster than would correspond to thermal equilibrium. A satisfactory explanation for this tendency is still lacking. Krey (1982) has recently suggested a simple picture which can account for our observed difference in specific heats. He suggests that, as the temperature is *increased*, the system performs 'Barkhausen jumps' from one metastable state to another with a

lower free energy (in zero magnetic field). At each jump a step should occur both in the magnetisation $M(T)$ and the internal energy $U(T)$ (see figure 3). If one assumes that the specific heat given by the slope of $U(T)$ between two successive 'Barkhausen jumps' is just the specific heat $C_{\Delta U}$ connected with thermal energy fluctuations and C is the temperature derivative of the smeared energy curve, it follows that

$$C > C_{\Delta U}$$

in agreement with our observation. A difficulty related to this picture is, however, that it would lead to a different result for the energy curve measured upon *cooling*, which is contrary to our observations. It should also be noted that a freezing step, as described in the analysis presented above, does not lead to a discontinuity of the internal energy.

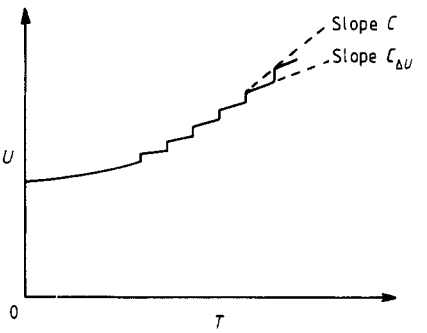

Figure 3. The staircase-like energy function $U(T)$ displaying 'Barkhausen jumps' (schematic).

It has been pointed out above that the margin of error attached to the value obtained for the residual experimental entropy $S_{\text{exp}}(0)$ is appreciable and that the thermodynamic significance of this quantity is in doubt because of the large width of the spin-glass transition region. On the other hand, for every particular cooling program which extends down to zero temperature, a well defined residual magnetic entropy $S(0)$ exists which is determined by the occupation probabilities $p_i(0)$ of different spin states at zero temperature:

$$S(0) = -k_B \sum_i p_i(0) \ln p_i(0). \tag{9}$$

It is this quantity that one would like to know. The question is how closely this 'statistical' residual entropy is approximated by the residual experimental entropy $S_{\text{exp}}(0)$ obtained from the specific heat measured in the computer experiment. It is now shown that a comparison of $S_{\text{exp}}(0)$ with an estimated upper bound to $S(0)$ suggests that both quantities agree within about a factor of two.

For the single-spin flip dynamics used in our MC calculations spin states occurring at absolute zero have to be stable against single-spin flips at $T = 0$. Such states are termed 'metastable states'. Therefore, in (9) the sum extends only over metastable states. If, for a given cooling rate, the MC trajectories end at zero temperature in metastable states with energies

$$E_i = U(0)[1 + O(N^{-1/2})], \tag{10}$$

which are close to the average internal energy $U(0)$, the density of metastable states $N_S(U(0))$ at this energy yields an upper limit to (9) for $S(0)$:

$$S(0) \leq k_B \ln N_S(U(0)). \tag{11}$$

The density of metastable states $N_S(E)$ for the infinite-range Ising spin glass has been calculated by Tanaka and Edwards (1980) and Bray and Moore (1981). For the short-range Edwards–Anderson model Bray and Moore (1981) calculated the first correction term in an expansion of $\ln N_S(E)$ in powers of z^{-1}, where z is the number of nearest neighbours. For the square lattice $z = 4$. In this case Bray and Moore's result should yield a good approximation to $N_S(E)$—except for the vicinity of the ground state energy E_0, in which we are mainly interested! The ground state energy of our model was determined by Morgenstern and Binder (1980) as

$$E_0 = (-1.31 \pm 0.01)\Delta J. \tag{12}$$

In their paper Morgenstern and Binder calculated thermodynamic equilibrium quantities by integrating over the entire spin space. Below E_0, the density of states is, of course, zero. From Bray and Moore's expansion one would obtain a finite density of metastable states at E_0, namely

$$(1/N) \ln N_S(E_0)|_{BM} \approx 0.11. \tag{13}$$

However, this result would imply that the spin glass has a finite residual entropy also in thermodynamic equilibrium, which contradicts Morgenstern and Binder's (1980) findings. It follows from the data of these authors that the equilibrium residual entropy is either zero or very small compared with the value given by (13). The reason why Bray and Moore's result is in error close to E_0 seems to be that the first two terms of the expansion in z^{-1} do not determine the ground state energy with sufficient accuracy. (Incidentally, Bray and Moore's calculation becomes invalid below a critical energy E_c which is close to, but lower than, our E_0.) For estimating the correct density of metastable states $N_S(E)$ near E_0, it is useful to derive the total density of spin states $N(E)$ from the equilibrium entropy $S_{eq}(T)$ as calculated by Morgenstern and Binder. From their result for low temperatures

$$S_{eq}(T) = 0.3Nk_B^2 T/\Delta J \tag{14}$$

which implies a linear specific heat, we deduce the equilibrium entropy as a function of residual energy $(E - E_0)$:

$$S_{eq}(E)/k_B N = [0.6(E - E_0)/(N\Delta J)]^{1/2}. \tag{15}$$

The equilibrium entropy is, on the other hand, determined by the total density of states $N(E)$ via

$$S_{eq}(E) = k_B \ln N(E) \tag{16}$$

if the energy spread ΔE of the macroscopic state is only of $O(\sqrt{N})$, as is normally the case. Combining (15) and (16), we obtain for the total density of states

$$(1/N) \ln N(E) = [0.6(E - E_0)/(N\Delta J)]^{1/2}. \tag{17}$$

In figure 4 this function (full line) is plotted together with the result for $N^{-1} \ln N_S(E)$ obtained from Bray and Moore's z^{-1} expansion (dotted line). The broken line in this figure represents an estimate for the density of metastable states which is consistent with the upper limits given by the two other curves. Here it was taken into account

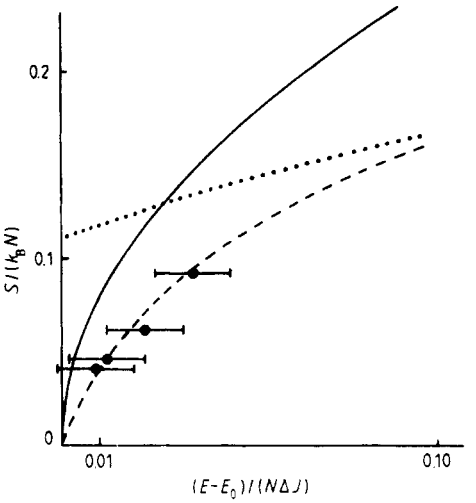

Figure 4. Various entropies as a function of residual energy. Full line: equilibrium entropy; dotted line: $N^{-1}\ln N_S(E)$ from z^{-1} expansion; broken line: estimate for $N^{-1}\ln N_S(E)$; points: Monte Carlo data for residual experimental entropy (see text).

that Bray and Moore's result should be fairly accurate for $(E-E_0)/(N\Delta J)\gtrsim 0.10$. It turns out (figure 4) that this estimate agrees within error with the MC data, obtained for different cooling rates, for the residual experimental entropy $S_{exp}(0)$ plotted against the residual energy $(U(0)-E_0)$. The error bars for these data are mainly due to the uncertainty of the ground state energy E_0 given by (12). Accordingly the residual experimental entropy is approximately equal to the upper limit (11) to $S(0)$:

$$S_{exp}(0)\approx k_B \ln N_S(U(0)). \tag{18}$$

Therefore, if the upper bound (11) is a good approximation to $S(0)$, the statistical residual entropy $S(0)$ and the residual experimental entropy $S_{exp}(0)$ are approximately equal. It seems very plausible indeed to assume that this latter condition is fulfilled. The condition is valid if a finite fraction r, which is independent of the size N of the system, of the metastable states at a given energy is accessible during the cooling process and has a finite occupation probability $p_i(0)$ at zero temperature. To violate the equality in relation (11) it would be necessary that, for example, only a fraction r of order $\exp(-\alpha N)$, where α is a positive constant, of the metastable states of energy $U(0)$ is reached at $T=0$. There is no obvious reason why such a selection of metastable states should take place in a random system of this kind.

The results and conclusions of this letter are now summarised. It has been inferred from the failure of the thermodynamic formula for energy fluctuations that the width of the spin-glass transition is appreciable. This casts doubt on the thermodynamic significance of the value obtained numerically for the residual experimental entropy, but a comparison with information derived from the equilibrium entropy curve and from a calculated density of metastable states suggests that our numerical results approximate the true residual entropy $S(0)$ within about a factor of two. It is proposed that $S(0)$ is determined by the residual energy $(U(0)-E_0)$ of the spin glass at $T=0$ and the density of metastable states $N_S(E)$ at this energy. The precise form of the $N_S(E)$ curve near the ground state energy E_0 has yet to be calculated.

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