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Ultrametricity in the infinite-range Ising spin glass

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Abstract. Monte Carlo simulations have been used to study the development of ultrametricity in the low-temperature phase of the infinite-range Sherrington–Kirkpatrick model of the Ising spin glass. Equilibrium configuration overlap data have been obtained for sizes N between 16 and 512 spins at the transition temperature $T = T_c$ and in the spin-glass phase at $T = 0.6T_c$. At the lower temperature, the data are consistent with the emergence, in the thermodynamic limit, of isosceles triangles formed by the mutual overlaps of three configurations, as predicted by Mezard and co-workers. Evidence for equilateral triangles is not clear and may require larger sizes. This behaviour is contrasted with the data at $T = T_c$, where all overlap distributions are found to scale with size in terms of a single exponent.

1. Introduction

The past few years have witnessed significant advances in our understanding of the low-temperature phase of the infinite-range model of spin glasses. The Sherrington–Kirkpatrick (SK) (1975) model, proposed originally as the mean-field limit of the Ising model of spin glasses (Edwards and Anderson 1975), iterated through a number of attempts (Thouless *et al* 1977, Bray and Moore 1978) before the broken replica symmetry solution was put forth (Parisi 1979, 1980a). The original solution of Parisi involved the generalisation of the concept of the spin-glass order parameter q to an order parameter function $q(x)$, of a once mysterious variable x which has been identified with a hierarchy of overlaps in the static description (Parisi 1980b) and a hierarchy of time scales in a dynamic description (Sompolinsky and Zippelius 1981, 1982, Sompolinsky 1981). Later, it became clear (Parisi 1983) that x is an integral of the probability distribution $P(q)$ of the spin-glass order parameter q , i.e. $dx/dq = P(q)$. $P(q)$ is defined in the following way. The system is not in a unique thermodynamic state (Young 1981, de Dominicis and Young 1983) but, in the statistical mechanics average, is in different states ‘ α ’ with probability P_α . If the magnetisation of site i when the system is constrained to be in state ‘ α ’ is m_i^α , then $P(q)$ is defined to be

$$P(q) = \left\langle \sum_{\alpha, \beta} P_\alpha P_\beta \delta(q - q^{\alpha\beta}) \right\rangle_J \quad (1)$$

where

$$q^{\alpha\beta} = \frac{1}{N} \sum_i m_i^\alpha m_i^\beta \quad (2)$$

is the ‘overlap’ between the magnetisation of states α and β , and $\langle \dots \rangle_J$ is an average over the quenched random-bond configuration.

Unlike the corresponding distribution of the order parameter in a system without disorder (e.g. the distribution $P(m)$ of magnetisation m for a ferromagnet), $P(q)$ does not reduce to a single delta function (modulo symmetry operations) even in the thermodynamic limit $N \rightarrow \infty$. Instead, $P(q)$ consists of a delta function at the Edwards–Anderson order parameter q_{EA} plus a continuous distribution below q_{EA} , going down to $q = 0$. A non-trivial $P(q)$ for $N \rightarrow \infty$ implies that the system is not in a unique thermodynamic state in the low-temperature phase. The Edwards–Anderson order parameter, q_{EA} measures ordering in a single state and is the same for all states while the continuous part of $P(q)$ comes from ‘overlaps’ between different states. Because a few states dominate the statistical sum, a number of quantities are not self-averaging in the thermodynamic limit (Mezard *et al* 1984a, b; Young *et al* 1984). Following these results was the discovery (Mezard *et al* 1984a, b) that the space of states $\{\alpha\}$ was ultrametric; namely, if one considers the overlaps $q_{\alpha\beta}$, $q_{\beta\gamma}$ and $q_{\gamma\alpha}$ between three pure states α , β and γ , then the smaller two are strictly equal in the thermodynamic limit. Thus the triangle whose sides are the three overlaps is isosceles. Furthermore, there is a finite probability (one quarter) of having all three equal (equilateral triangle), an occurrence which has zero probability for randomly chosen triangles. The isosceles triangle is a direct consequence of the replica breaking scheme and implies a hierarchical development of the free-energy minima (valleys) below the spin-glass transition temperature. The equilateral triangle is based on the more subtle property of the weights of the various valleys (Mezard *et al* 1987). These results follow without further assumptions from the replica method and Parisi’s scheme. However, a linear stability analysis of the broken replica symmetry solution (de Dominicis and Kondor 1983), while yielding no instabilities, has shown a large number of marginal directions (zero-mass modes), and a non-linear stability analysis has not been performed. In other words, while the Parisi solution is shown to be extremal, it is not proved with certainty that it is *the* low-temperature phase. Indeed, there have been very recent challenges to the Parisi solution (Horner 1986, 1987). Thus it would be interesting to check its predictions using other techniques (e.g. numerical simulations). In this paper, we describe such numerical simulations, with emphasis on testing the predictions of ultrametricity. A preliminary report on some of these results has appeared elsewhere (Bhatt and Young 1986). Searches for ultrametricity have been made in other models (Sourlas 1984, Kirkpatrick and Toulouse 1985, Solla *et al* 1986, Mezard *et al* 1987) and a review article has appeared recently (Rammal *et al* 1986).

2. Computational details

We have performed Monte Carlo simulations on the SK model in zero magnetic field for a sequence of sizes ranging from $N = 16$ spins to $N = 512$ spins at the spin-glass transition temperature T_c , and at a temperature $T = 0.6T_c$. The Hamiltonian for the system is

$$H = - \sum_{ij} J_{ij} S_i S_j \quad (3)$$

where $S_i = \pm 1$ are Ising spins and the sum in equation (3) is over all pairs. J_{ij} are quenched random variables with a probability distribution

$$P(J_{ij}) = [(N-1)/2\pi]^{1/2} \exp[-(N-1)J_{ij}^2/2] \quad (4)$$

i.e. a Gaussian distribution with mean zero and variance $(N-1)^{-1}$ chosen to give a mean field $T_c = 1$.

The sequence of sizes studied have been found previously (Bhatt and Young 1985) to be large enough to confirm the T_c and mean-field exponents via a finite-size scaling analysis. Evidence for a non-trivial $P(q)$ in the low-temperature phase (Young 1983) was seen in even smaller sizes ($N < 192$), although the convergence towards the infinite- N limit was somewhat slow. $P(q)$ has also been analysed by others (Parga *et al* 1984) using a different method, which is approximate.

For each size, we run in parallel *three* copies S_i^α ($\alpha = 1-3$) of the system with the same *bond* configuration and accumulate data with 40–2000 different bond realisations depending on size. The copies are started with *independent random* initial configurations (characteristic of infinite temperature) and allowed to come to equilibrium in a time t_0 and measurements are made over the next $2t_0-10t_0$. The method of ensuring equilibration has been described previously (Bhatt and Young 1985, 1988). Basically, it consists of ascertaining whether the spin-glass susceptibility obtained from different copies

$$\chi_{SG}^a(t_0) = \frac{1}{3N\tau} \left\langle \sum_{\alpha>\beta} \sum_{t=1}^{\tau} \left[\sum_i S_i^\alpha(t_0+t) S_i^\beta(t_0+t) \right]^2 \right\rangle_J \tag{5}$$

equals that obtained from the same copy:

$$\chi_{SG}^b(t_0) = \frac{1}{3N} \left\langle \sum_{\alpha} \left[\sum_i S_i^\alpha(t_0) S_i^\alpha(2t_0) \right]^2 \right\rangle_J \tag{6}$$

within statistical errors. It is found that equation (5) underestimates the true χ_{SG} while equation (6) overestimates it if t_0 is not long enough. Both of course converge to the true χ_{SG} for long enough t_0 , where $\chi_{SG} = N^{-1} \sum_{i,j} \langle S_i S_j \rangle_T^2$ and $\langle \dots \rangle_T$ denotes a thermal average for a given realisation of the bonds J_{ij} and $\langle \dots \rangle_J$ indicates an average over the bond distribution.

We have looked at various quantities related to the spin overlap between different copies:

$$Q_{\alpha\beta}(t) = \frac{1}{N} \sum_i S_i^\alpha(t_0+t) S_i^\beta(t_0+t). \tag{7}$$

One is the usual order parameter probability distribution

$$P_N(q) = \frac{1}{3\tau} \sum_{\alpha>\beta} \sum_{t=1}^{\tau} \langle \delta[q - |Q_{\alpha\beta}(t)|] \rangle_J \tag{8}$$

where we have restricted ourselves to $q > 0$, noting that $P_N(-q) = P_N(q)$ in zero field in equilibrium. Note that $P_N(q)$ is defined in terms of microscopic states whereas $P(q)$ (equation (1)) involves the properties of thermodynamics states. However, it is straightforward to show (Young 1985) that the two agree in the thermodynamic limit, i.e.

$$\lim_{N \rightarrow \infty} P_N(q) = P(q). \tag{9}$$

In fact, our criterion for equilibration only guarantees the convergence of even moments of $P_N(q)$; the vanishing of the odd moments can only be achieved on the longer time scale of flipping the entire ensemble. Instead, our procedure puts that in by hand.

To study the correlations among the overlaps $Q_{\alpha\beta}$, we look at probability distributions of *differences* between the three instantaneous overlaps $Q_{12}(t)$, $Q_{23}(t)$ and $Q_{31}(t)$. We first label them q_1, q_2, q_3 in decreasing order of their magnitudes and, if necessary,

reverse one of the sets of spin configurations $S_i^1(t)$, $S_i^2(t)$ or $S_i^3(t)$ to make q_1 and q_2 positive. Thus $q_1 \geq q_2 \geq |q_3| \geq 0$. Mathematically, this can be expressed as

$$q_1 = \max(|Q_{12}|, |Q_{23}|, |Q_{31}|) \quad (10a)$$

$$q_3 = \text{sgn}(Q_{12} Q_{23} Q_{31}) \min(|Q_{12}|, |Q_{23}|, |Q_{31}|) \quad (10b)$$

$$q_2 = |Q_{12}| + |Q_{23}| + |Q_{31}| - q_1 - |q_3|. \quad (10c)$$

According to Mezard *et al* (1984a), $\langle q_3 \rangle$ is guaranteed to be positive and in fact equal to $\langle q_2 \rangle$ in the thermodynamic limit. Consequently, we look at the probability distribution

$$\Phi_I(\delta q) = \sum_t \delta[q_2(t) - q_3(t) - \delta q] \quad (11)$$

(the subscript I stands for the isosceles triangles supposed to emerge as $N \rightarrow \infty$). As for $P_N(q)$, we calculate $\Phi_I(\delta q)$ from microscopic states but this goes over to the corresponding quantity defined in terms of thermodynamic states for $N \rightarrow \infty$. The latter is predicted (Mezard *et al* 1984a, b) to be $\delta(\delta q)$. Consequently, $\Phi_I(\delta q)$ should tend to $\delta(\delta q)$, i.e. a delta function at the origin, in the thermodynamic limit. For finite but large N , therefore, one may expect $\Phi_I(\delta q)$ to be strongly peaked near $\delta q = 0$. However, care must be taken to distinguish between effects due to the predicted ultrametric topology and other effects which can look rather similar. For example, one can define the Hamming distance $d_{\alpha\beta}^H$ between two microscopic states α and β by

$$d_{\alpha\beta}^H = \frac{1}{2} \left(1 - \frac{1}{N} \sum_i S_i^\alpha S_i^\beta \right). \quad (12)$$

This is just N^{-1} times the number of spins which have different orientations in the two states. The Hamming distances satisfy triangular inequalities

$$d_{\alpha\beta}^H \leq d_{\beta\gamma}^H + d_{\gamma\alpha}^H \quad (13)$$

which imposes the restriction

$$\delta q = q_2 - q_3 \leq 1 - q_1. \quad (14)$$

Thus, for $q_1 \rightarrow 1$, δq is guaranteed to be small for reasons having nothing to do with ultrametricity. In fact, for $N \rightarrow \infty$, where one can define thermodynamic states and $P(q) = 0$ for q_{EA} there is a more stringent restriction. Consider the N -dimensional vectors formed from the site magnetisations m_i^α for various thermodynamic states. One can construct the Euclidean distance $d_{\alpha\beta}^E$ between two states, where clearly

$$d_{\alpha\beta}^E = [2(q_{EA} - q_{\alpha\beta})]^{1/2}. \quad (15)$$

The triangular inequality then gives

$$(q_{EA} - q_1)^{1/2} \geq (q_{EA} - q_3)^{1/2} - (q_{EA} - q_2)^{1/2} \quad (16)$$

and so $\delta q \rightarrow 0$ as $q_1 \rightarrow q_{EA}$. Hence it is necessary to study $\Phi_I(\delta q)$ for q_1 significantly less than q_{EA} , although q_1 cannot be too small as otherwise most of the data will be discarded and the statistics will be poor. Furthermore, we study $\Phi_I(\delta q)$ as a function of sample size as a means of separating effects due to triangle inequalities (which are presumably less size independent) than those due to ultrametricity.

To check for equilateral triangles, we have looked at the variation in the distribution of the quantity $\Delta q \equiv 2q_1 - q_2 - q_3$, i.e.

$$\Phi_E(\Delta q) = \sum_i \delta[2q_1(t) - q_2(t) - q_3(t) - \Delta q]. \tag{17}$$

Equilateral triangles formed by the $d_{\alpha\beta}^H$ would have equal q -values and would consequently contribute a delta function to $\Phi_E(\Delta q)$ at $\Delta q = 0$. However, unlike $\Phi_1(\delta q)$, which was supposed to be a pure delta function at the origin as $N \rightarrow \infty$, $\Phi_E(\Delta q)$ is predicted to have an extra continuous part due to the non-equilateral isosceles triangles. In fact, using the calculated distribution of three mutual overlaps (Mezard *et al* 1984a, b),

$$\begin{aligned} P(q_1, q_2, q_3) = & \frac{1}{2}P(q_1)x(q_1)\delta(q_1 - q_2)\delta(q_2 - q_3) \\ & + \frac{1}{2}[P(q_1)P(q_2)\theta(q_1 - q_2)\delta(q_2 - q_3) \\ & + P(q_2)P(q_3)\theta(q_2 - q_3)\delta(q_3 - q_1) \\ & + P(q_3)P(q_1)\theta(q_3 - q_1)\delta(q_1 - q_2)] \end{aligned} \tag{18}$$

one may show that

$$\Phi_E(\Delta q) = \frac{1}{4}\delta(\Delta q) + \frac{3}{4}P(q_1 - \Delta q/2)/x(q_1) \tag{19}$$

where $x(q)$ is the Parisi replica symmetry breaking variable, with $P(q) \equiv dx/dq$, and $x(0) = 0$.

Since we shall discuss the size dependence of our results, it is useful, at this point, to discuss what is known about finite-size effects in the SK model. For $T > T_c$ and large N , $P_N(q)$ is Gaussian, and the width is $(\chi_{SG}/N)^{1/2}$ since χ_{SG} is, by definition, N times the second moment of $P_N(q)$. At T_c , $P_N(q)$ will have a different shape whose width will no longer vary as $N^{-1/2}$ because χ_{SG} diverges for $N \rightarrow \infty$. In fact, one expects (Bray and Moore 1979) that $\chi_{SG} \propto N^{1/3}$ and so the width varies as $N^{-1/3}$. The natural finite-size scaling *ansatz* for $P_N(q)$ is then

$$P_N(q) = N^{1/3} \bar{P}(N^{1/3}q) \quad (T = T_c). \tag{20}$$

For $T < T_c$, $P(q)$ has a delta function at $q = q_{EA}$ due to the self-overlap of a single valley. This will become a peak of finite width in $P_N(q)$ due to fluctuations between microscopic states belonging to a single valley. It appears that each thermodynamic state is ‘marginal’ (Bray and Moore 1979, Sompolinsky 1981) so that for example the spin-glass susceptibility of a single valley, χ_{SG}^α , defined by

$$\chi_{SG}^\alpha = \frac{1}{N} \sum_{i,j} (\langle S_i S_j \rangle_T^\alpha - \langle S_i \rangle_T^\alpha \langle S_j \rangle_T^\alpha) \tag{21}$$

will diverge everywhere in the ordered phase. Here $\langle \dots \rangle_T^\alpha$ denotes a partial average in state ‘ α ’. We expect that the width of the peak in $P_N(q)$ around $q = q_{EA}$ will be $(\chi_{SG}^\alpha/N)^{1/2}$. It has been argued (Bray and Moore 1979) that $\chi_{SG}^\alpha \propto N^{1/3}$, the same as at T_c , so that again the width is proportional to $N^{-1/3}$. This can also be inferred from recent calculations of χ_{SG}^α (de Dominicis and Kondor 1986). They compute the Gaussian fluctuations about the mean-field solution but for a finite-range model obtaining $\chi_{SG}^\alpha(\mathbf{k}) = k^{-2}$, where \mathbf{k} is the wavevector, both at and below T_c . For a system of linear dimension L , this would become L^2 (because the smallest \mathbf{k} in the box is proportional to

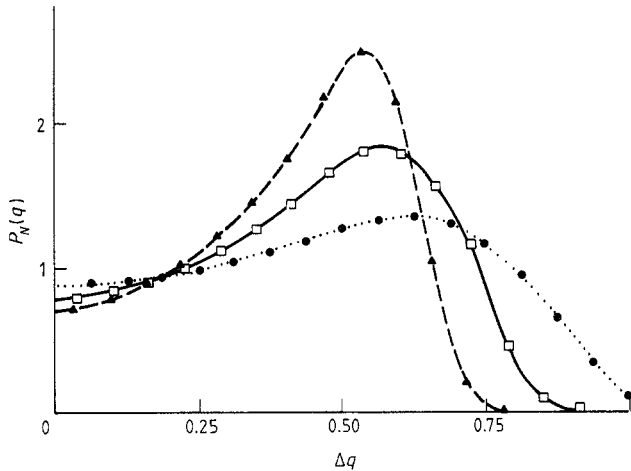


Figure 1. Order parameter distribution function $P_N(q)$ for $N = 32$ (\bullet , \cdots), $N = 128$ (\square , ---) and $N = 512$ (\blacktriangle , ---).

L^{-1}) and, to convert this to the N dependence of the infinite-range model using $N = L^d$, one should use the upper critical dimension $d = d_u = 6$ (Bray and Moore 1979, Binder *et al* 1985). This gives the $N^{1/3}$ dependence. We expect any distribution whose width in q comes from fluctuations in a single thermodynamic state will have a width which varies asymptotically as $N^{-1/3}$ both below and at T_c . Above T_c , one would have the conventional $N^{-1/2}$ dependence.

3. Results and discussion

3.1. The low-temperature phase ($T = 0.6T_c$)

Figure 1 shows the distribution of overlaps $P_N(q)$ for sizes $N = 32, 128$ and 512 at $T = 0.6T_c$. As can be seen, there is a gradual evolution of a peak in $P_N(q)$ with increasing size at the Edwards–Anderson order parameter q_{EA} . The approximate formula $q_{EA} = 1 - 2(T/T_c)^2 + T/T_c$, which correctly gives the first three terms in an expansion away from T_c and also gives correctly a quadratic variation with T as $T \rightarrow 0$ with about the correct coefficient, yields an estimate $q_{EA} = 0.496$. In agreement with previous work (Young 1983) at $T = 0.4T_c$, we find a tail extending down to $q = 0$. The somewhat more pronounced size dependence in our results than in the previous work is not unexpected as the temperature here ($0.6T_c$) is closer to T_c . For the largest size $N = 512$ the apparent reduction in $P_N(q)$ at low q is within statistical error. (Since $P_N(q)$ is not self-averaging, it is subject to large sample-to-sample fluctuations.)

We plot in figure 2(a) the distribution $\Phi_1(\delta q)$ using the data within the interval $q_1 = \frac{1}{2} \pm \frac{1}{2}$ for sizes $N = 32, 128$ and 512 . (It is necessary to take a finite window for q_1 , rather than a fixed value, so that statistics do not deteriorate catastrophically as size increases.) As can be seen, the distribution narrows dramatically with size. However, this value of q_1 is almost equal to q_{EA} for the infinite system, although it is at the lower end of the peak in $P_N(q)$ for the sizes studied. Consequently, for large N , such that the peak is close to q_{EA} but the width is not smaller than the difference between this q_1 and q_{EA} , two copies would be in the *same* thermodynamic state, and the distribution $\Phi_1(\delta q)$ would be a measure of the width of the peak in $P_N(q)$ rather than ultrametricity. While it is unlikely that the sharpening of the peak in $P_N(q)$ is the *entire* cause of the narrowing of $\Phi_1(\delta q)$,

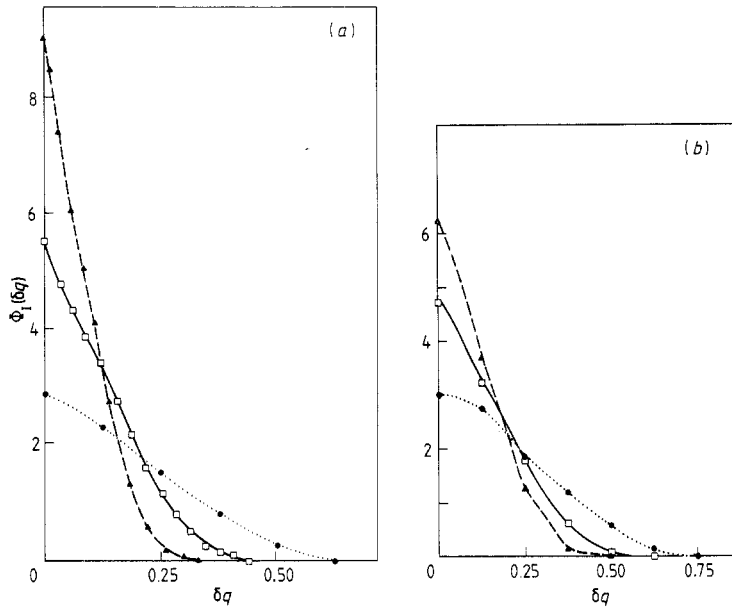


Figure 2. Distribution function $\Phi_1(\delta q)$ for (a) $q_1 = \frac{1}{2}$ and (b) $q_1 = \frac{3}{8}$, indicating the growth of ‘isosceles triangles’ with size at $T = 0.6T_c$, for $N = 32$ (\bullet , \cdots), $N = 128$ (\square , —) and $N = 512$ (\blacktriangle , ---).

since q_1 is significantly below the peak in $P_N(q)$ even for our largest size, we have obtained the same distribution for a different window of $q_1 = \frac{3}{8} \pm \frac{1}{32}$, and this is shown in figure 2(b). The narrowing is not as fast but is nevertheless present; this value of q_1 is well below q_{EA} for the infinite system and is clearly in the tail of $P_N(q)$ for the sizes studied. The difference between the results for the two q_1 could be because for $q_1 = \frac{1}{2}$, there is additional narrowing effect due to the sharpening up of the $P_N(q)$ as discussed above. Alternatively, because the extent of the distribution of $\delta q (= q_2 - q_3)$ is bounded by the magnitude of q_1 (since q_2 and q_3 are smaller than it, by definition), there may be some saturation effects for small N and low q_1 . This would make the apparent dependence of the width of Φ_1 on N weaker at low N , resulting in an overall weaker dependence for our range of N for $q_1 = \frac{3}{8}$ than it would be as $N \rightarrow \infty$. We are unable to say which of the two is the correct interpretation. For a smaller value of q_1 ($q_1 = \frac{1}{4}$), we find even smaller variation with size, which could be suggestive evidence in favour of the latter scenario. However, in this case our results have large statistical errors because of the smaller sampling size and cannot be overly relied on.

Figure 3 shows in a double-logarithmic plot the variation in the first moment of $P_N(q)$ and of $\Phi_1(\delta q)$ for $q_1 = \frac{1}{2}$ and $\frac{3}{8}$ with N for sizes $N = 16\text{--}512$. The variation in the width of Φ_1 with N is consistent with a power-law decrease N^{-x} with $x \approx 0.33$ for $q_1 = \frac{1}{2}$ and $x = 0.25$ for $q_1 = \frac{3}{8}$. In contrast, the first moment of $P_N(q)$ varies little with N and appears to be saturating at the Parisi value

$$\int q(x) dx = 1 - \frac{T}{T_c} \tag{22}$$

which is 0.4 for our temperature. The second moment of $P_N(q)$, also shown in figure 3, varies somewhat more with N but is consistent with extrapolation to the value

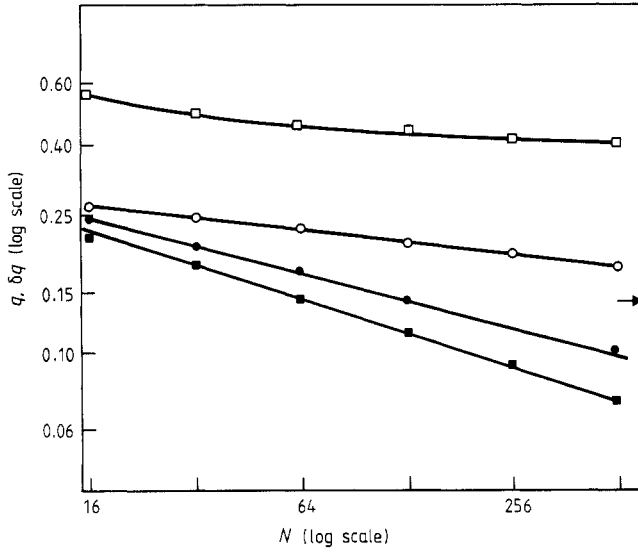


Figure 3. Double-logarithmic plot of the first moment $\langle |q| \rangle$ (□) and second moment $(\langle q^2 \rangle - \langle |q| \rangle^2)^{1/2}$ (○) of $P_N(q)$, and the first moment $\langle \delta q \rangle$ of $\Phi_1(\delta q)$ for $q_1 = \frac{1}{2}$ (■) and $q = \frac{3}{8}$ (●) against N ($N = 16-512$). The arrow denotes the value of the second moment of $P(q)$ as $N \rightarrow \infty$, calculated approximately.

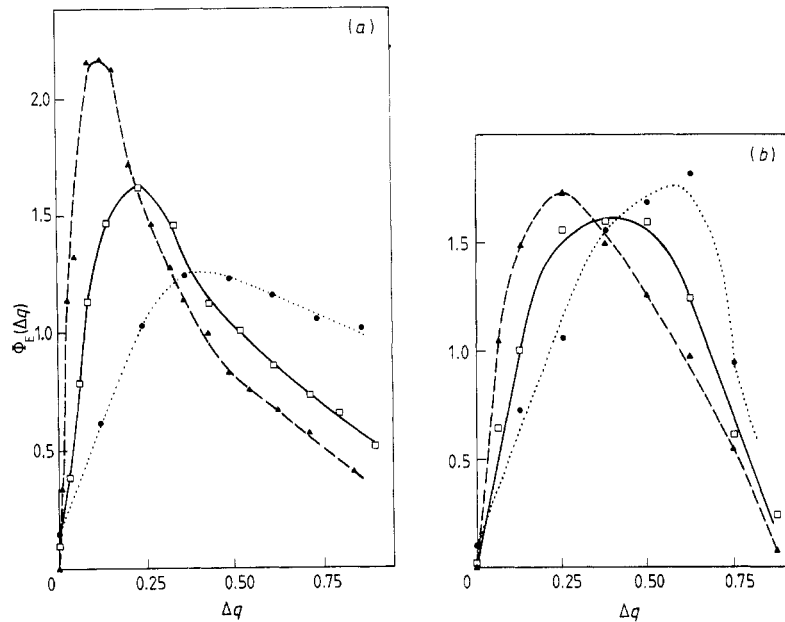


Figure 4. Distribution function $\Phi_E(\Delta q)$ for (a) $q_1 = \frac{1}{2}$ and (b) $q_1 = \frac{3}{8}$, looking for the growth of 'equilateral triangles' with size at $T = 0.6T_c$: $N = 32$ (●, \cdots), $N = 128$ (□, ---) and $N = 512$ (▲, ---).

$(\langle q^2 \rangle - \langle |q| \rangle^2)^{1/2} \approx 0.14$, which is obtained by replacing $\langle q^2 \rangle$ by the SK solution (Sherrington and Kirkpatrick 1975). (This is probably not a bad approximation, since $\langle q^2 \rangle = 1 - 2T|U|/T_c^2$ for the SK model, and the energy U for the Parisi solution differs very little from the SK solution.)

We now look at the distribution of $\Delta q = 2q_1 - q_2 - q_3$ to see the evidence for equilateral triangles. Figure 4(a) plots the distribution $\Phi_E(\Delta q)$ with $q_1 = \frac{1}{2}$ for the same

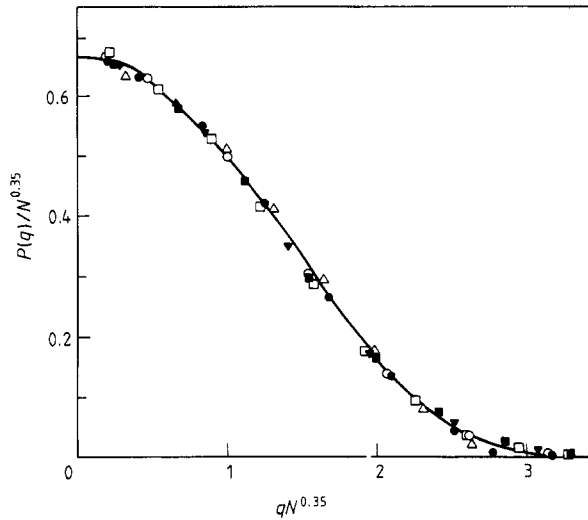


Figure 5. Universal scaling plot at $T = T_c$ of the order parameter distribution function: \triangle , $N = 16$; \bullet , $N = 32$; \circ , $N = 64$; \square , $N = 128$; \blacksquare , $N = 256$; \blacktriangledown , $N = 512$.

sequence of sizes $N = 32, 128$ and 512 . There appears to be a shift in weight towards low Δq , consistent with the results of Mezard *et al* (1984a, b) that $\Phi_E(\Delta q)$ has a delta function contribution at $\Delta q = 0$. However, unlike $\Phi_I(\delta q)$, $\Phi_E(\Delta q)$ has an additional component out to large Δq , as expected from equation (19) on the basis of the Parisi solution, because of which the results cannot be analysed more quantitatively without resorting to theory. However, one clear complicating feature is that, for large finite sizes N , $\Phi_E(0)$ appears to be zero, linearly with a slope proportional to N ; so, if it does approach a delta function as $N \rightarrow \infty$, the approach is somewhat more complex than in the case of $\Phi_I(\delta q)$. (This should be contrasted with the result for infinite N based on the Parisi solution, equation (19), which has a finite intercept at $\Delta q = 0$, in addition to the δ -function.) Figure 4(b) for $q_1 = \frac{3}{8}$ demonstrates this difference even more dramatically. We have evidence from the data at T_c that finite-size corrections to $\Phi_E(\Delta q)$ are larger than for $\Phi_I(\delta q)$ or $P_N(q)$; consequently, results for larger sizes, or finite- N corrections to the Parisi result, are necessary, before an adequate test of this prediction can be made.

3.2. The critical temperature ($T = T_c$)

The ultrametric correlations are supposed to be a property of the low-temperature phase; if, so, they should not be seen at T_c , where there is no replica symmetry breaking. At T_c , the Edwards–Anderson order parameter $q_{EA} \rightarrow 0$ in the thermodynamic limit; consequently, one has to scale the overlaps by $qN^{1/3}$ to search for any possible ultrametricity within the narrowing distributions of q , δq and Δq . Because the whole distribution shrinks towards the origin as $N \rightarrow \infty$, we have used data for *all* q_1 rather than a *fixed* q_1 in obtaining the distribution of δq and Δq . Figure 5 shows the scaled plot of $P(qN^\lambda)/N^\lambda$ against qN^λ with $\lambda = 0.35$, and all sizes $N = 16$ – 512 fall within our error bars on one universal plot, except for small deviations for $N = 16$ and perhaps $N = 32$. The value $\lambda = 0.35$ is within acceptable bounds of the expected value $\lambda = \frac{1}{3}$, considering that finite-size scaling corrections for T_c (Bhatt and Young 1985) ranging from 10% ($N = 32$ – 128) to 3% ($N = 128$ – 512).

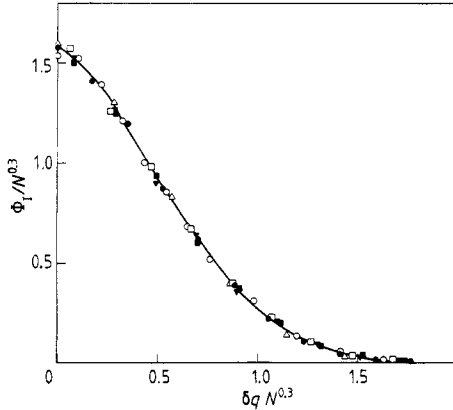


Figure 6. Universal scaling plot at $T = T_c$ of the distribution $\Phi_I(\delta q)$ (see text): \triangle , $N = 16$; \bullet , $N = 32$; \circ , $N = 64$; \square , $N = 128$; \blacksquare , $N = 256$; \blacktriangledown , $N = 512$.

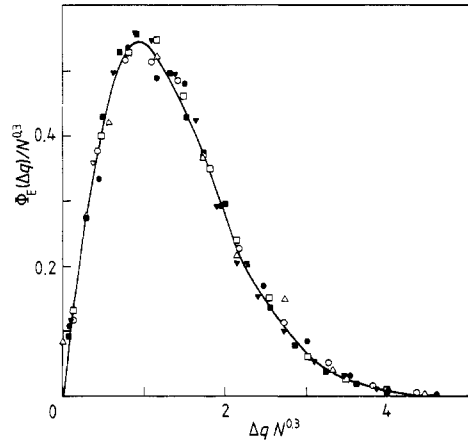


Figure 7. Universal scaling plot at $T = T_c$ of the distribution $\Phi_E(\Delta q)$ (see text): \triangle , $N = 16$; \bullet , $N = 32$; \circ , $N = 64$; \square , $N = 128$; \blacksquare , $N = 256$; \blacktriangledown , $N = 512$.

Figure 6 shows the corresponding plot for $\Phi_I(\delta q)$, i.e. $N^{-\lambda}\Phi_I(\delta q N^\lambda)$ against $\delta q N^\lambda$. Once again the data for all sizes $N = 16$ –512 collapse onto a single universal plot with $\lambda = 0.3$, which is also within acceptable limits of the result $\lambda = \frac{1}{3}$ expected on the basis of a single order parameter exponent. If there was any tendency towards ultrametricity near T_c as has been suggested for the three-dimensional short-range spin glass for small sizes (Sourlas 1984) then, with increasing N , δq should have scaled to zero faster than q and the λ -value for the scaling plot for $\Phi_I(\delta q)$ in figure 6 should have been higher than that for $P_N(q)$ in figure 5. Our best fits show instead that within our resolution the two are the same.

Finally the scaling plot for equilateral triangles $\Phi_E(\Delta q N^\lambda)/N^\lambda$ against $\Delta q N^\lambda$ with $\lambda = 0.3$ is shown in figure 7, and again the data fall onto one universal plot. Here, however, we see greater finite-size effects and a systematic trend for the deviation for smaller sizes ($N = 64, 32$ and 16). This universal scaling plot shows, as the previous plot did, that any ultrametricity that is present in a SK spin glass is a property of the *low-temperature phase*.

4. Conclusions

We have studied, via Monte Carlo simulation, the infinite-range (SK) Ising spin glass at the transition temperature T_c and, in the spin-glass phase ($T = 0.6T_c$), for sizes $N = 16$ –512. By running three copies of each sample (same size and bond configurations) in parallel, we probe various quantities related to the three mutual overlaps. Our results are consistent with earlier work (Young 1983) which indicated a non-trivial overlap distribution $P_N(q)$ for large N . By looking at the size dependence of the distribution $\Phi_I(\delta q)$ of the difference between the smaller two of the overlaps, we find that the distribution becomes more peaked at $\delta q = 0$, with increasing N . However, the dependence on N varies with the value chosen for the largest overlap q_1 , within our range of sizes. The strongest variation in the width is proportional to $N^{-0.33}$, for $q_1 \approx q_{EA}$, may be enhanced owing to narrowing effects of the peak in $P_N(q)$ as N increases. The weaker

variation, e.g. that proportional to $N^{-0.25}$ at $q_1 \approx 0.75q_{EA}$, and even slower for $q_1 \approx 0.5q_{EA}$, may be somewhat reduced because of saturation effects at small N . Because of these complications, we cannot give a definitive value for the intrinsic variations in the $N \rightarrow \infty$ limit. Nevertheless, our results are consistent with the expectation on the basis of the Parisi solution that $\Phi_I(\delta q)$ scales to a delta function at $\delta q = 0$ in the thermodynamic limit.

We have also looked at the size dependence of the distribution $\Phi_E(\Delta q)$ where Δq is the difference between twice the maximum overlap and the sum of the two smaller overlaps (out of the three). Our results indicate a growth in weight at small Δq with increasing N , as expected with the Parisi solution which gives a finite probability of all three overlaps equal and hence a delta function in $\Phi_E(\Delta q)$ at $\Delta q = 0$. However, here the dependence q_1 is even larger, and so larger sizes and theoretical input of finite-size corrections are necessary before a quantitative analysis can be made. One other worry is that, unlike the predictions of Mezard *et al* (1984a, b) for the thermodynamic limit $N \rightarrow \infty$, the smallest overlap q_3 does not turn out to be always positive for our N , and the incidence of negative q_3 (5–10% for our q_1) does not decrease significantly with increasing N in our range.

By contrast, our results at $T = T_c$ imply that all distributions $P_N(q)$, $\Phi_I(\delta q)$ and $\Phi_E(\Delta q)$ scale similarly with N consistent with the expected result.

In conclusion, we have attempted the most systematic and detailed investigation of ultrametricity in the infinite-range Ising spin glass to date. The strongest evidence in its favour appears to be the narrowing of the distribution $\Phi_I(\delta q)$, indicating the emergence of isosceles triangles. Unfortunately, even in this case, a definitive analysis is not possible, because of complications due to finite-size effects. The evidence for equilateral triangles is rather weak, and the distribution $\Phi_E(\Delta q)$ is far from that expected from the Parisi theory. Given the difficulties that we have found in seeing ultrametricity in the SK model, where there are strong theoretical arguments that it occurs, we feel that claims made for ultrametricity in other models should be carefully checked to see whether other factors such as triangle inequalities or a peaked distribution $P(q)$ might be influencing the data.

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