Ordering Temperatures and Critical Exponents in Ising Spin Glasses

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We propose a numerical criterion which can be used to obtain accurate and reliable values of the ordering temperatures and critical exponents of spin glasses. Using this method we find a value of the ordering temperature for the $\pm J$ Ising spin glass in three dimensions which is definitely nonzero and in good agreement with previous estimates. We show that the critical exponents of three-dimensional Ising spin glasses do not obey the usual universality rules. [S0031-9007(96)01198-2]

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The full explanation of the universality rules for critical exponents in second order transitions through the renormalization group theory is one of the most impressive achievements of statistical physics. The universality rules for such transitions state that the critical exponents depend only on the space dimension d and a few basic parameters: the number of order parameter components n, the symmetry, and the range of the Hamiltonian [1]. No other parameters are pertinent. In fact, it is known that there are exceptions to universality—in certain two-dimensional ($2d$) Ising systems with regular frustration, the critical exponents vary continuously with the value of a control parameter [2]. As far as we are aware, no results of this type have been reported in any three-dimensional ($3d$) family of Ising systems; it has been tacitly assumed that nonuniversality is very exceptional.

As compared to standard second order transitions, the situation concerning Ising spin glasses (ISGs) is much less clear; indeed the history of ISG simulations has been plagued by technical difficulties associated with long relaxation times. For two decades the very existence of a finite temperature transition in the $3d$ ISG has been hotly contested; as it is obviously essential to have a reliable value of the ordering temperature before obtaining accurate critical exponent estimates, it has been difficult to make stringent numerical tests of universality in $3d$ ISGs.

We will present a numerical criterion which can in favorable cases provide precise and reliable values for the ordering temperature T_g and for the critical exponents of a spin glass, with a moderate level of computational effort. If an independent estimate of the ordering temperature is available the criterion leads to a convenient method for estimating the exponents. We study $3d$ ISGs with various sets of interactions, and we conclude from the data that the $3d \pm J$ interaction ISG has a well-defined nonzero T_g which can be estimated accurately, and that universality in the usual sense does not hold in $3d$ ISGs.

It would appear probable that glassy transitions in general have a much richer critical behavior than conventional second order transitions.

Thus, technically, the most difficult problem in numerical ISG studies is the correct identification of the transition temperature T_g. For the $3d$ ISG with random $\pm J$ near neighbor interactions on a simple cubic lattice, which has been the subject of a considerable amount of work, T_g has been estimated in two ways. Ogielski [3] studied in massive simulations the divergence of the spin glass susceptibility, correlation length, and relaxation time of the autocorrelation function

$$q(t) = \langle S_i(t) S_i(0) \rangle \tag{1}$$

in order to estimate T_g and the critical exponents. However, his analysis has been questioned because of the possibility of ambiguities in the manner of identifying a divergence, if nonconventional temperature dependencies are invoked [4]. Bhatt and Young [5] used a finite size scaling technique; they measured the Binder cumulant for the fluctuations of the equilibrium autocorrelation function

$$g_L = \frac{1}{2}\left[3 - \frac{\langle q^4 \rangle}{\langle q^2 \rangle^2}\right] \tag{2}$$

as a function of sample size L. The curves $g_L(T)$ for different L should all intersect at T_g; in the $3d \pm J$ ISG case the curves indeed intersected but did not appear to fan out below the apparent T_g. Only recently have intensive numerical studies shown that a weak fanning out at low temperatures really does occur [6,7]. Even with results of high statistical accuracy at hand, Kawashima and Young [6] give a number of caveats concerning the interpretation of their own data.

We will describe an alternative criterion for determining T_g. First, scaling rules [3] tell us that for a large sample in thermal equilibrium at T_g the relaxation of the autocorrelation function takes the form

$$q(t) = \lambda t^{-x} \tag{3}$$

with the exponent x related to the standard static and dynamic exponents η and z through

$$x = \frac{d - 2 + \eta}{2z}. \tag{4}$$

Second, the out of equilibrium relaxation of two randomly chosen replicas A and B of the same sample towards equilibrium at T_g depends on another combination

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of the same exponents [8]. The out of equilibrium spin glass susceptibility is defined as

$$\chi_{SG}^{l}(t) = [\langle S_i^A(t) S_i^B(t) \rangle^2], \tag{5}$$

and it increases with time as t^h with

$$h = \frac{2 - \eta}{z}. \tag{6}$$

Suppose we take $\{T_i\}$, a series of trial values for T_g; from measurements of x and h on large samples at each T_i we can deduce from Eqs. (4) and (6) a set of apparent or effective exponents

$$\eta_1(T) = \frac{4x - h(d - 2)}{2x + h}, \tag{7}$$

$$z(T) = \frac{d}{2x + h}. \tag{8}$$

Finally, in another set of simulations on the same system at different (small) sample sizes L, from standard finite size scaling rules [5] for the fluctuations in the autocorrelation function in equilibrium at T_g we have

$$L^{d-2}\langle q^2 \rangle \propto L^{-\eta}. \tag{9}$$

If we again take a series of trial values of T_g and fit the results using this form at each T_i we will obtain a second series of apparent exponent values $\eta_2(T)$. (This type of fit will only be appropriate close to and below T_g; at higher T another factor appears on the right-hand side [5].)

We now plot $\eta_1(T)$ and $\eta_2(T)$ against T; for consistency the curves must intersect at the point (η, T_g), which represents the true critical exponent η and ordering temperature T_g of the system. At this temperature and this temperature only the functional forms of Eqs. (3), (6), and (9) should be exact; at neighboring temperatures these forms are only approximate, but close to T_g they will be adequate to parametrize the numerical data. Once T_g is fixed by the intersection we can obtain z using the $z(T)$ curve given above, and with known η and T_g we can go on to fit $\langle q^2 \rangle$ data for temperatures above T_g to obtain the exponent ν. From scaling relations, once we dispose of η and ν all other static exponents are determined.

We show in Fig. 1 estimates for $\eta_1(T)$ and $\eta_2(T)$ for the $3d$ $\pm J$ ISG calculated using data taken from the literature: $x(T)$ from [3], $h(T)$ from [8,9], and the spin glass susceptibilities for different assumed values of T_g ($T_g = 1.0$ from the data given in [5], $T_g = 1.11$ from [6], and $T_g = 1.175$ from [3]). There is a well-defined crossing point with $T_g = 1.165 \pm 0.01$ and $\eta = -0.245 \pm 0.02$. Using the curve for $z(T)$ from Eq, (8) we estimate $z = 6.0 \pm 0.2$.

The values obtained in this way are at least as precise as previous estimates and are very close to the central values given by Ogielski [3] ($T_g = 1.175 \pm 0.025$, $\eta = -0.22 \pm 0.05$, $z = 6.0 \pm 0.8$), corroborating his analysis. On the other hand, the T_g is marginally outside the error bars quoted by Kawashima and Young ($T_g = 1.11 \pm 0.04$) who use extensive Binder cumulant data [6]. The difficulty in applying this latter method to the $3d$ $\pm J$ ISG case is that the $g_L(T)$ curves lie very close together below T_g so the intersection point is sensitive to small changes in individual g_L curves. Even with extreme statistical accuracy, small corrections to finite size scaling (invoked as a possibility in [6]) can change the apparent position of the intersection point significantly. The results of Ref. [6] could be rendered consistent with the present analysis if the g_L values for the smallest samples studied were affected by corrections to finite size scaling at the 1% level.

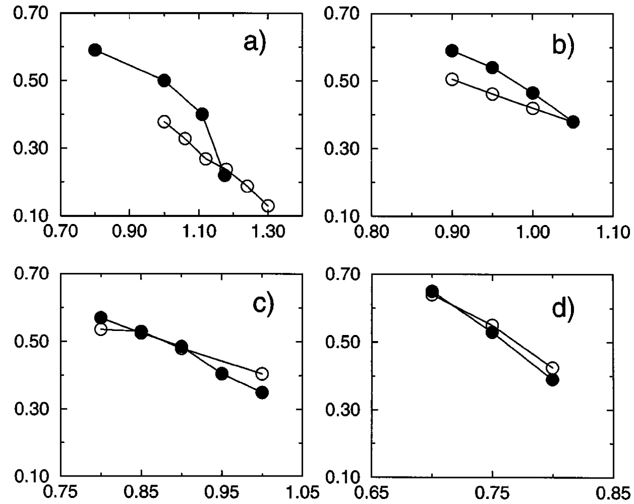

FIG. 1. η_1 ($\circ$) and η_2 ($\bullet$) vs T for various distributions. (a) $\pm J$, (b) uniform, (c) Gaussian, and (d) decreasing exponential. Note that the scale on the x axis is different for each plot. Error bars on individual η points are about ± 0.02.

The present method is much less sensitive to problems of systematics than are either of the other techniques outlined above. First, both x and h are determined using "large" samples, so finite size corrections should be unimportant [8,9]. Second, h is measured out of equilibrium and so is not subject to the problems of long equilibration times. The fact that no preparatory anneal is required also means that the measurements are economical in computer time. The measurements of x need careful equilibration, but systematic tests using successively longer preliminary anneals allow one to obtain reliable values. Numerical data [3,9] show that in ISGs $q(t)$ already takes on the asymptotic form, Eq. (3), from quite early times $t \simeq 2$ MCS (Monte Carlo steps), and that sample to sample variations in the values of x are small so extensive averaging over very large numbers of samples (an essential condition for good g_L data) is unnecessary. Thus the curve $\eta_1(T)$ can be established accurately with moderate numerical effort and minimal systematic error. For the finite size scaling data from which $\eta_2(T)$ is deduced, thorough equilibration is necessary, but by studying pairs of replicas [5] and again testing with increasing anneal times it is easier to obtain accurate values of $\langle q^2(t) \rangle$ than the combination of moments which constitute the Binder cumulant. Again, the sample to sample variability is much less for $\langle q^2(t)\rangle$ than for the Binder cumulant. In the $3d$ $\pm J$ ISG the two curves $\eta_1(T)$ and $\eta_2(T)$ intersect cleanly, Fig. 1, so the determination of the crossing point should not be very sensitive to minor deviations from scaling or small statistical uncertainties. Finally, no hypothesis is made concerning the way divergences occur except the essential assumption that standard scaling rules (as opposed to universality rules) hold. The excellent overall agreement between Ogielski's estimates [3] and the present ones gives considerable confidence in the general coherence of the standard scaling approach and appear to make any exotic scaling assumption unnecessary.

We therefore consider that both $\eta_i(T)$ curves can be calculated with little in the way of disguised systematic errors; as they stand, the T_g and exponent values that we quote should not only be precise but reliable.

We have made further simulations on another $3d$ ISG with $\pm J$ interactions; this is the fully frustrated system with 20% random bond disorder that we studied in [10]. We already established an accurate value of T_g ($T_g = 0.96$) for this spin glass from Binder cumulant measurements, and we now have measured the exponents x and h at T_g together with an estimate of η from the spin glass susceptibility (see Table I). The data are very consistent with each other and lead to an η value which is less negative and a z value which is smaller as compared with those of the standard $\pm J$ ISG. This difference already indicates the nonuniversality of these two exponents in $3d$ ISGs.

We have also carried out extensive simulations on $3d$ ISG systems with different sets of near neighbor interactions. For the $3d$ ISGs with near neighbor uniform, Gaussian, and decreasing exponential interactions (see [11] for the definitions of the distributions with the correct normalizations), the data are shown in Fig. 1. Simulations were done on samples with $L = 16$ for x, $L = 10$ for h, and samples from $L = 2$ to 6 for $\langle q^2(t)\rangle$. Careful anneals were carried out where appropriate, checked by the prescription given in [5]. At each temperature, 10 samples were used for x, 500 for h, and 2000 to 200 depending on L for $\langle q^2(t)\rangle$. We estimate that the $\eta_1(T)$ curves are on large enough samples for there to be virtually no finite size correction, so the values can be taken as definitive (apart from statistical errors), but measurements on larger samples could modify the $\eta_2(T)$ curves marginally. It can be seen that the $\eta(T)$ curves again cross cleanly for the uniform case with a more negative η than for the $\pm J$ case. However, for the Gaussian and exponential cases it turns out that the two curves are much more similar to each other making it difficult to identify T_g precisely; for these distributions we have to fall back on an alternative method to estimate T_g.

The Migdal-Kadanoff (MK) scaling approach is known to give reasonable values of the ordering temperature for Ising spin glasses [12–14]. We have followed the particular method used by Curado and Meunier [14] but with improved statistical accuracy. It turns out that with a scale factor $b = 2$ the MK estimate for the $3d$ $\pm J$ ISG T_g is 1.16 ± 0.01, precisely the same as the value we have obtained above from the simulations. This perfect agreement is certainly fortuitous (though in $4d$, where the MK method should be much poorer, the disagreement in T_g between the $b = 2$ MK estimate and an accurate simulation value is only 15% [15]), but we argue that as agreement happens to be excellent for the $\pm J$ case, if we apply the same method with the same scale factor b to other $3d$ ISGs with different sets of interactions, we should obtain T_g estimates which should again be very close to the real values. We obtain MK T_g values which are 1.00, 0.88, and 0.72 for the uniform, Gaussian, and exponential distributions, respectively [15]. The uniform distribution value is in good agreement with the simulation value, and the other two T_g values are within the range of T, where the simulation curves for $\eta_1(T)$ and $\eta_2(T)$ overlap. The Gaussian T_g and η are in good agreement with earlier estimates [5]. Putting uncertainties at ± 0.05 for possible systematic errors in the Gaussian and exponential MK T_g estimates, we obtain the set of exponent estimates shown in Table I.

According to the usual universality rules, the form of the interaction distribution should not be a pertinent parameter as concerns the critical exponents. Here we find that $3d$ ISG systems which differ only by this distribution function show quite different η and z values, Table I. The results indicate a breakdown of conventional universality in $3d$ ISGs.

TABLE I. Temperature of transiton and critical exponents for several distributions. The distributions are in order (i) random $\pm J$ interactions, (ii) fully frustrated lattice with 20% disorder [10], (iii) random uniformly distributed interactions, (iv) random Gaussian interactions, and (v) random decreasing exponential interactions.

System	T_g	$x(T_g)$	$h(T_g)$	η	z
$\pm J$	1.165 ± 0.01	0.064	0.38	-0.245 ± 0.02	6.0 ± 0.2
FFd0.2	0.96 ± 0.02	0.091	0.437	-0.12 ± 0.02	4.85 ± 0.3
U	1.05 ± 0.03	0.054	0.41	-0.375 ± 0.03	5.8 ± 0.5
G	0.88 ± 0.05	0.035	0.355	-0.50 ± 0.04	7.1 ± 0.6
Exp	0.72 ± 0.05	0.02	0.275	-0.62 ± 0.12	9.5 ± 0.7

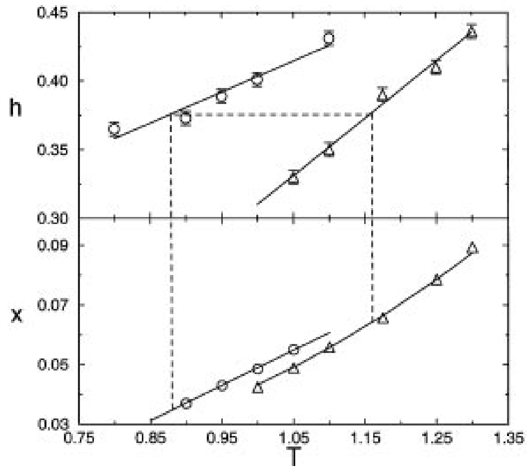

FIG. 2. $h(T)$ and $x(T)$ for $\pm J$ ($\triangle$) and uniform ($\circ$) distributions. The temperature scale is common. The dashed line corresponds to the example given in the text.

In order to show that the apparent nonuniversality is not an artifact, we will turn back to the raw x and h data for the $\pm J$ and uniform cases. In Fig. 2 we have plotted the values of these parameters as a function of T; the error bars are about ± 0.005 for h and ± 0.002 for x.If universality holds

$$h(T_g(U)) \equiv h(T_g(J)), \qquad (10)$$

$$x(T_g(U)) \equiv x(T_g(J)). \qquad (11)$$

By inspection, whatever trial value T^* we choose for $T_g(J)$ within the generous limits $T^* = 1.0$ to 1.3 provided by the figure, the relation (10) leads us to a $T_g^*(U)$ such that $x(T_g^*(U))$ is considerably smaller than $x(T_g^*(J))$. For instance, with $T_g^*(J) = 1.16$, $T_g^*(U) = 0.88$, $x(T_g^*(J)) = 0.064$, and $x(T_g^*(U)) = 0.036$. The data cannot satisfy (10) and (11) simultaneously, demonstrating nonuniversality.

For the $2d$ regularly frustrated systems which show continuous variation of critical exponents, the breakdown of universality is necessarily associated with the existence of a marginal operator [16], and it has been pointed out that when breakdown occurs, it does so in Ising systems having more than two ground states [17] and hence with n, the number of components of the order parameter, greater than 1 [18]. On the Parisi image of finite dimension ISGs [19], n is essentially infinite; it would be of interest to identify possible marginal operators. We can note that in the regularly frustrated $2d$ systems quoted above, ν varies continuously but η is constant so "weak universality" [20] still holds. This is not the case for the randomly frustrated systems we have studied.

It would appear that universality breakdown could be much more prevalent than was suspected, and it may well be the rule rather than the exception at spin glass or glass transitions.

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[1] S.K. Ma, *Modern Theory of Critical Phenomena* (Benjamin, New York, 1976).
[2] R.J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, London, 1982); R.H. Swendsen and S. Krinsky, Phys. Rev. Lett. **43**, 177 (1979); K. Minami and M. Suzuki, Physica (Amsterdam) **195A**, 457 (1993); M. Kolesik and L. Samaj, J. Stat. Phys. **72**, 1203 (1993).
[3] A.T. Ogielski and I. Morgenstern, Phys. Rev. Lett. **54**, 928 (1985); A.T. Ogielski, Phys. Rev. B **32**, 7384 (1985).
[4] E. Marinari, G. Parisi, and F. Ritort, J. Phys. A **27**, 2687 (1994).
[5] R.N. Bhatt and A.P. Young, Phys. Rev. B **37**, 5606 (1988).
[6] N. Kawashima and A.P. Young, Phys. Rev. B **53**, R484 (1996).
[7] K. Hukushima and K. Nemoto (unpublished).
[8] D.A. Huse, Phys. Rev. B **40**, 304 (1989).
[9] R.E. Blundell, K. Humayun, and A.J. Bray, J. Phys. A **25**, L733 (1992); F. Wang, M. Suzuki, and N. Kawashima (unpublished).
[10] I.A. Campbell and L. Bernardi, Phys. Rev. B **52**, R9819 (1995).
[11] L. Bernardi and I.A. Campbell, Phys. Rev. B **49**, 728 (1994); Phys. Rev. B **52**, 12 501 (1995).
[12] C. Jayaprakash, C. Chalupa, and M. Wortis, Phys. Rev. B **15**, 1495 (1977).
[13] B.W. Southern, A.P. Young, and P. Pfeuty, J. Phys. C **12**, 683 (1979).
[14] E.M.F. Curado and J.L. Meunier, Physica (Amsterdam) **149A**, 164 (1988).
[15] S. Prakash and I.A. Campbell (unpublished).
[16] L.P. Kadanoff and F.J. Wegner, Phys. Rev. B **4**, 3989 (1971).
[17] K. Jungling, J. Phys C **9**, L1 (1976).
[18] S. Krinski and D. Mukamel, Phys. Rev. B **16**, 2313 (1977).
[19] G. Parisi, Physica (Amsterdam) **194A**, 28 (1993).
[20] M. Suzuki, Prog. Theor. Phys. **51**, 1992 (1974).