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Finite-size-scaling study of the simple cubic three-state Potts glass: Possible lower critical dimension $d=3$

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For small lattices with linear dimension L ranging from $L=3$ to $L=8$ we obtain the distribution function $P(q)$ of the overlap q between two real replicas of the three-state Potts-glass model with symmetric nearest-neighbor interaction with a Gaussian distribution. A finite-size-scaling analysis suggests a zero-temperature transition to occur with an exponentially diverging correlation length $\xi_{SG} \sim \exp(C/T^{\sigma})$. This implies that $d=3$ is the lower critical dimension.

With an improved understanding[1] of Ising spin glasses, the Potts-glass model is receiving more attention. The Potts glass is not only a model for anisotropic orientational glasses, but may also provide a first step towards modeling the glass transition of structural glasses. Indeed there exist[2] intriguing analogies between the mean-field theory of the Potts-glass and the mode-coupling approach[3] to the glass transition. Furthermore, the mean-field theory of the Potts glass[4] differs markedly from the mean-field theory of the spin glass.[5,6] In addition, many features of short-range spin glasses differ qualitatively[7,8] from the mean-field predictions. It is therefore interesting to ask about the properties of short-range Potts glasses: to what extent they are different from spin glasses and from mean-field predictions. A question of paramount importance is the value of the lower critical dimension d_l, below which the transition is at zero temperature. For Ising spin glasses d_l lies between 2 and 3,[8-11] so a finite-temperature transition occurs in $d=3$ but not for $d=2$, while for vector spin glasses $d_l \approx 4$, so $T_c=0$ even for $d=3$. For isotropic orientational glasses the transition is also believed[12] to occur at $T=0$ in $d=3$, whereas for Potts glasses the situation is less clear. This Rapid Communication attempts to determine whether T_c is finite or not for the three-state Potts glass in $d=3$ dimensions by combining Monte Carlo simulations with a finite-size scaling analysis. Further details of the analysis are given in Ref. 13. The model Hamiltonian is given by[14]

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij}\mathbf{s}_i \cdot \mathbf{s}_j \, , \tag{1}$$

where the $\mathbf{s}_i$ are equal to any of the set of p basis vectors, $\mathbf{S}^{\alpha}$, with the property that $(\mathbf{S}^{\alpha})^2=1$ and $\mathbf{S}^{\alpha}\cdot\mathbf{S}^{\beta} = -1/(p-1)$ if $\alpha\neq\beta$. Here we specialize to the case of $p=3$. The sites i lie on a simple cubic lattice with $N=L^3$ sites and the sum is over all nearest-neighbor pairs (i,j). An energy J_{ij} is gained if the neighboring sites (i,j) are in the same state. Each J_{ij} is a quenched random variable drawn from a symmetric Gaussian distribution. We follow the usual normalization of the interactions in the Potts model by setting $[J_{ij}^2]_{av} = p/(p-1)$, where $[\cdots]_{av}$ denotes a bond average. In these units the mean-field transition temperature is given by $T_c^{MF}=\sqrt{z}/p$, where z is the coordination number. For the present case of $z=6$, $p=3$ this gives $T_c^{MF}=0.8165$. Periodic boundary conditions are applied in all directions to avoid surface effects.

As in earlier finite-size scaling studies of spin glasses[10] we analyze the order parameter distribution $P(q)$ and its moments. The order parameter is defined in terms of the overlap between the configurations of two copies (replicas) of the system with identical interactions and no coupling between them. After dropping t_0 sweeps for equilibration and running for an additional t_m sweeps, where $t_m \geq t_0$, for measurement, we compute the instantaneous mutual overlap between the configurations of the replicas defined by

$$q^{\mu\nu}(t) = \frac{1}{N}\sum_{i=1}^{N} s_{i,1}^{\mu}(t_0+t)s_{i,2}^{\nu}(t_0+t) \, , \tag{2}$$

where μ and ν refer to components of the Potts vectors. In order to avoid unnecessarily long relaxation times and to obtain good statistics, it is necessary that the order parameter q be invariant under global symmetries of the Hamiltonian. Hence we define $q(t)$ by

$$q(t) = \left(\sum_{\mu,\nu}[q^{\mu\nu}(t)]^2\right)^{1/2} , \tag{3}$$

which is clearly invariant under simultaneous rotations of all the vectors in either replica. The order parameter distribution is then calculated from

$$P(q) = \frac{1}{N_m}\left[\sum_{t=1}^{N_m}\delta(q-q(t))\right]_{av} , \tag{4}$$

where N_m denotes the number of measurements performed.

To check whether the equilibration time t_0 is sufficient for the system to be in equilibrium, we used the technique developed by one of us[10] for spin glasses. Namely, in addition to computing $P(q)$ from the overlap between two replicas, we also compute a distribution $\tilde{P}(q)$ obtained from the overlap between the configurations of a single replica at times t_0 and $2t_0$. More precisely we compute

$$\tilde{q}^{\mu\nu}(t_0) = \frac{1}{N}\sum_{i=1}^{N} s_i^\mu(t_0) s_i^\nu(2t_0) ,$$

and the distribution $\tilde{P}(q)$ is defined by

$$\tilde{P}(q) = [\delta(q - \tilde{q}(t_0))]_{\text{av}} ,$$

where $\tilde{q}(t_0) = \{\sum_{\mu,\nu}[\tilde{q}^{\mu\nu}(t_0)]^2\}^{1/2}$. As discussed in Ref. 10 $P(q)$ and $\tilde{P}(q)$ should agree only if the simulation is long enough that both give the equilibrium result. Runs where the answers disagreed by more than the estimated errors were, therefore, discarded.

The dramatically increasing relaxation times limited our simulations to rather small lattices of linear sizes ranging from $L = 3$ to $L = 8$. For the biggest size, 4×10^6 Monte Carlo steps (MCS) were needed at the lowest temperature ($T = 0.3$), where we discarded $t_0 = 2\times10^6$ MCS for equilibration. Between times t_0 and $2t_0$ typically a few hundred measurements were performed. The number of samples in the configurational average varied between 400 and 500.

We now focus on the finite-size behavior of the moments $\langle q^n\rangle = \int q^n P(q)dq$, where we note that $\langle q^2\rangle$ is simply related to the spin-glass susceptibility by $\chi_{\text{SG}} = N\langle q^2\rangle = N^{-1}\sum_{i,j}[\langle \mathbf{s}_i\cdot\mathbf{s}_j\rangle_T^2]_{\text{av}}$, where $\langle\cdots\rangle_T$ denotes a statistical-mechanics average for a given bond configuration. The standard finite-size scaling assumption is

$$\langle q^n\rangle = L^{-n(d-2+\eta)/2} f_n(L^{1/\nu}(T-T_c)) , \tag{5}$$

where η describes the decay of correlations at T_c, ν is the correlation-length exponent, and the f_n are scaling functions. Equation (5) implies that the power of L in front of the scaling function cancel for the "renormalized coupling" g_L defined by[10,15]

$$g_L = 3 - 2\frac{\langle q^4\rangle}{\langle q^2\rangle^2} = \tilde{g}(L^{1/\nu}(T-T_c)) . \tag{6}$$

As defined, $g_L \to 0$ as $L\to\infty$ above T_c because in this limit the 4 components $q^{\mu\nu}$ have independent Gaussian fluctuations, and $g_L \to 1$ as $L\to\infty$ below T_c, since $\langle q^4\rangle = \langle q^2\rangle^2$ in this limit. Hence, data for g_L for different sizes should *intersect* at T_c. This provides a convenient method for locating the transition temperature. As written, Eq. (5) is appropriate for cases where the spin-glass correlation length ξ_{SG} diverges with a power of $(T-T_c)$, where a finite T_c would indicate a situation with $d > d_l$, while $T_c = 0$ would indicate $d < d_l$, i.e.,

$$\xi_{\text{SG}} \sim \begin{cases} (T-T_c)^{-\nu}, & d > d_l , \\ T^{-\nu}, & d < d_l ! . \end{cases} \tag{7}$$

In addition, we wish to consider the possibility that the system is at its lower critical dimension, in which case the correlation length diverges exponentially, i.e.,

$$\xi_{\text{SG}} \sim \exp(CT^{-\sigma}),\ d = d_l , \tag{8}$$

where McMillan's scaling theory[16] predicts $\sigma = 2$. Note that for all cases, χ_{SG} is related to ξ_{SG} by $\chi_{\text{SG}} \sim \xi_{\text{SG}}^{2-\eta}$. Note also that for $d \le d_l$, one has $\eta = 2-d$ if the ground state is nondegenerate.[15] To allow for this more general case one should reexpress Eq. (6) as

$$g_L = \tilde{g}(L/\xi_{\text{SG}}(T)) \tag{9}$$

and similarly

$$\chi_{\text{SG}} = L^{2-\eta}\tilde{\chi}(L/\xi_{\text{SG}}(T)) . \tag{10}$$

The first step in analyzing the data is to search for T_c from the intersection of the curves for g_L for different sizes. Our results for g_L are plotted in Fig. 1 from which it is clear that T_c must either be zero or very low compared with the mean-field value of 0.8165. In fact, it seems clear that the data cannot merge for $T > 0.15$ so T_c must be less than this value and, hence, we can improve on the upper bound of $T_c < 0.23$ given in Ref. 17. Since it would be a coincidence for T_c to be nonzero yet extremely small compared with T_c^{MF}, Fig. 1 already suggests that $T_c = 0$. Further evidence for this will be presented below.

Assuming that T_c is zero we need to distinguish whether there is a power law or exponential divergence of ξ_{SG} and χ_{SG} as $T\to0$. To do so we have chosen a procedure which does not enforce the asymptotic form for ξ_{SG} in Eqs. (7) and (8), but rather tries to obtain it from the data itself. To do this we determine the value of $\chi_{\text{SG}}(T) \equiv \chi_{\text{SG}}(\infty,T)$ for each temperature by extrapolation, and a characteristic length $l(T)$ by requiring that the data for $\chi_{\text{SG}}(L,T)/\chi_{\text{SG}}(T)$ collapses onto a single curve when plotted against $L/l(T)$. We obviously use the normalization that $\chi_{\text{SG}}(L,T)/\chi_{\text{SG}}(T) = 1$ as $L/l(T)\to\infty$, but the overall normalization of $l(T)$ is arbitrary. Finite-size scaling tells us, however, that $l(T)$ is proportional to $\xi_{\text{SG}}(T)$ whatever choice is made for the normalization. The result of this analysis is plotted in Fig. 2 while Fig. 3(a) shows a log-log plot of the obtained values of $\ln[l(T)]$ against T. The scaling of the data in Fig. 2 clearly works well, particularly bearing in mind that a

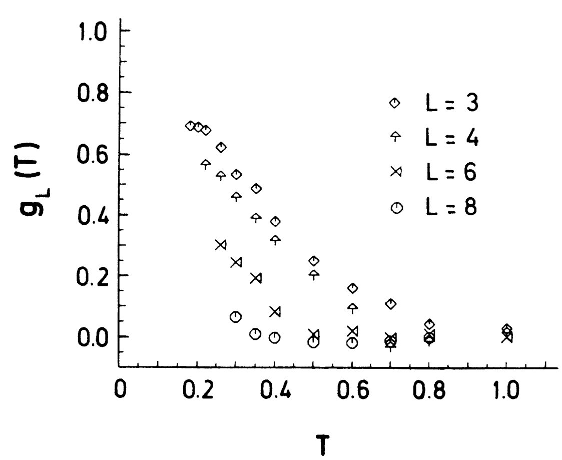

FIG. 1. Reduced cumulant g_L plotted vs T for different lattice sizes. These results were obtained from Monte Carlo runs with up to 4×10^6 MCS (for $L = 8$ at $T = 0.3$) and typically an average over 400–500 bond configurations were performed. Note that g_L is defined such that $g_{L\to\infty} = 0$ in the disordered phase, $g_{L\to\infty} = 1$ in a phase with nonzero order parameter, while curves for g_L for different sizes should intersect at a critical point.

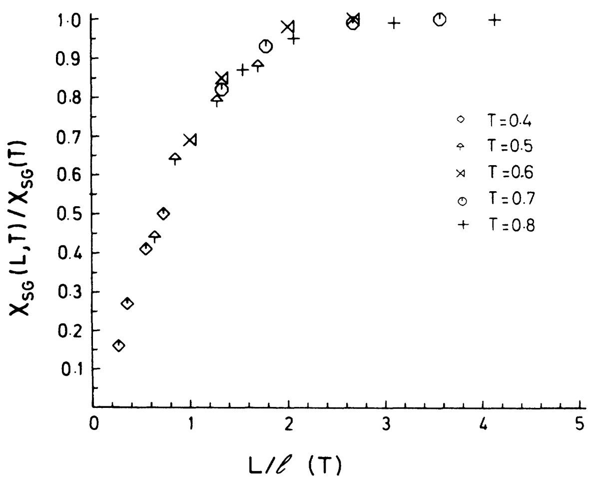

FIG. 2. Scaling plot of $\chi_{SG}(L,T)/\chi_{SG}(T)$ against the scaled variable $L(T)/l(T)$. Here $\chi_{SG}(T)$ has been adjusted to get the fit and the characteristic lengths $l(T)$ are fit parameters.

linear rather than a logarithmic scale is used. The results for the characteristic length $l(T)$ in Fig. 3(a) are consistent with the behavior in Eq. (8) expected at the lower critical dimension and the slope of -1.97 is very close to the theoretical value -2. Figure 3(b) is a log-log plot of χ_{SG} against $l(T)$. The slope, which should equal $2-\eta$, is found to be 1.5 and so $\eta=0.5$.

As noted above, one expects $\eta=-1$ if $T_c=0$ and the ground state is nondegenerate. Since η is very different from this we conclude that the ground state is degenerate as for a Potts antiferromagnet.[14]

Clearly our results cannot rule out a very small but finite T_c, but this seems less likely than the picture presented above of an exponential divergence at $T=0$ implying that 3 is the lower critical dimension for the Potts glass. A recent domain wall calculation[18] finds $T_c=0$ for the $\pm J$ distribution in three dimensions, but $T_c>0$ for the Gaussian model. However, in both cases the value found for the zero-temperature exponent is very small. Hence, given the small sizes studied, we believe that their results are consistent with $d_l=3$ for both distributions and are therefore consistent with our conclusions.

To conclude, we have shown that the behavior of the Potts glasses in three dimensions is different from that of Ising spin glasses. Whereas the latter have a finite transition temperature with power-law divergencies, data for the Potts glass at intermediate temperatures fits much better the hypothesis that $T_c=0$ with exponential divergencies as $T\rightarrow 0$. It would be very valuable to test for these differences experimentally.

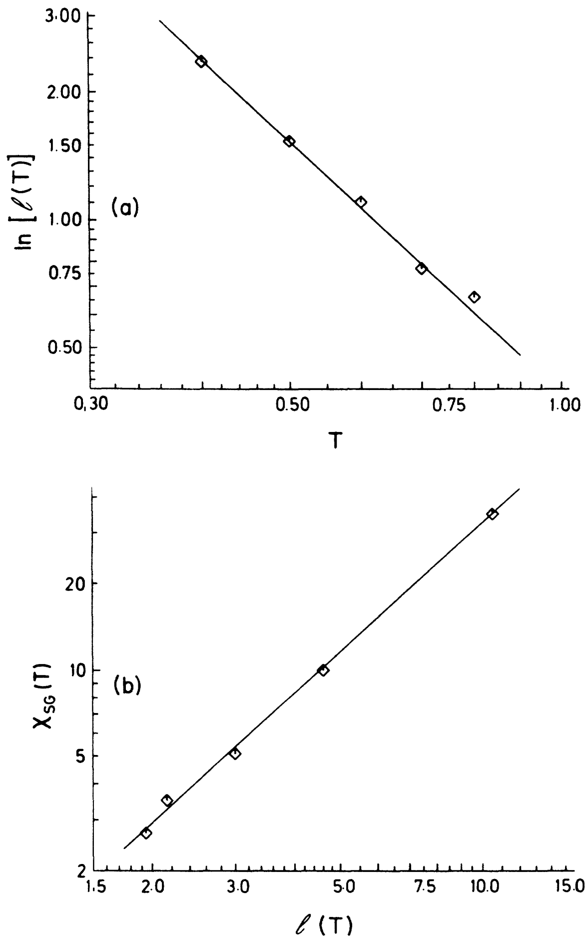

FIG. 3. Log-log plot of $\ln[l(T)]$ vs T. The straight line has slope -1.97, close to the value of -2 expected for a system at its lower critical dimension. (b) Log-log plot of $\chi_{SG}(T)$ vs $l(T)$. $l(T)$ is proportional to $\xi_{SG}(T)$, so the slope should be $2-\eta$, independent of the value of the lower critical dimension. From the data we find the slope to be 1.5. This is to be contrasted with the value of three expected if $T_c=0$ and the ground state is nondegenerate. Hence we infer that this model has a highly degenerate ground state.

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