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Evidence of a one-step replica symmetry breaking in a three-dimensional Potts glass model

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We study a seven-state Potts glass model in three dimensions with first-, second-, and third-nearest-neighbor interactions with a bimodal distribution of couplings by Monte Carlo simulations. Our results show the existence of a spin-glass transition at a finite temperature T_c, a discontinuous jump of an order parameter at T_c without latent heat, and a nontrivial structure in the order parameter distribution below T_c. They are compatible with one-step replica symmetry breaking.

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Introduction. Mean-field spin-glass models without time-reversal symmetry have been studied by many researchers over the last few decades. A class of models that differ greatly from the Sherrington-Kirkpatrick Ising spin glass [1], such as the p-spin model and p-state Potts glass model [2,3], exhibits two distinct phase transitions [4,5]. One is a dynamical phase transition at a temperature T_d, below which an exponentially large number of metastable states emerge, and a spin autocorrelation function does not decay to zero in the long time limit. The latter is a consequence of ergodicity breaking. The other is a purely thermodynamic transition at $T_c < T_d$, which is called the random first-order transition (RFOT). At T_c, the entropy associated with the metastable states vanishes, and an order parameter emerges discontinuously without latent heat; below T_c, the replica symmetry is broken at the one-step level. A particularly intriguing fact is that at the mean-field level, the dynamical equations for a time correlation function near T_d in these models are formally identical to the mode-coupling equations in the theory of structural glass transitions. This fact suggests a potentially deep connection between spin-glass models with quenched disorder and structural glasses with no quenched disorder [6–12]. All of the phenomena described above are called the RFOT scenario in the study of the glass transition and are speculated to be a promising candidate for a mean-field description of the glass transition. Thus, the mean-field spin-glass theory has been developed in great detail, revealing that some spin-glass models represent a prototypical model of the RFOT scenario, at least at the mean-field level [5,13,14].

One of the main issues to be addressed is whether these mean-field predictions are valid in finite dimensions in which fluctuations must be taken into account. A straightforward way to investigate the effect of fluctuation is to examine finite-dimensional spin-glass models that display the RFOT in the mean-field limit. Extensive Monte Carlo studies of the p-state Potts glass models in a three-dimensional cubic lattice have clarified the existence of the spin-glass transition at a finite temperature for $p \leqslant 6$ [15–17]. However, their properties are somewhat compatible with those of a continuous transition in the Ising spin-glass model, and no clear remnants of the RFOT have been found. In the mean-field theory, the discontinuity of the order parameter and also the difference between T_d and T_c grow with the number of states in the p-state Potts glass model [18,19]. Hence, it might be likely that the RFOT, if any, could be found in Potts glass models with relatively large p in finite dimensions. In addition, for such a large value of p, it is necessary to make most of the couplings antiferromagnetic to prevent ferromagnetic ordering. On the other hand, as pointed out in Ref. [20], when most of the couplings are antiferromagnetic, Potts glass models on any finite connectivity lattice are unfrustrated for large values of p, in the sense that these couplings are easily satisfied in the ground state. Thus, no glassy ordering is expected because the frustration is considered to be a key ingredient of the glassy behavior. Indeed, Brangian *et al.* found that there was no glassy phase in the ten-state Potts glass model with a bimodal distribution of the couplings and a small fraction of ferromagnetic couplings [21]. Thus, it is difficult to simultaneously avoid ferromagnetic ordering and maintain the frustration for Potts glass models with a large p on finite connectivity lattices. In particular, in the three-dimensional Potts glass model with only nearest-neighbor interactions, the low connectivity ($c = 6$) makes it difficult to meet this requirement.

To avoid the above difficulties, we propose a Potts glass model with not only the nearest-neighbor couplings, but also second- and third-nearest-neighbor couplings, on a three-dimensional cubic lattice. Although this model has only short-range interactions, such a high connectivity could yield frustration even in the antiferromagnetic case and even for large p. Using Monte Carlo simulations of the p-state Potts glass model with $p = 7$, we obtained the following results: (1) This model shows a static spin-glass transition at a finite temperature $T_c/J = 0.421(3)$ in the units of the Boltzmann constant, with the correlation length exponent $\nu = 0.68(9)$. (2) At T_c, the order parameter appears discontinuously, but no latent heat exists. (3) Below T_c, the order parameter distribution has a bimodal structure.

Model and numerical details. The p-state Potts glass model we studied is defined by the Hamiltonian

$$\mathcal{H}_{\mathcal{J}}(\sigma) = -\sum_{(i,j)} J_{ij}\delta(\sigma_i,\sigma_j), \tag{1}$$

where the Potts spin σ_i on site i takes $0,1,\ldots,p-1$, and the summation is over the nearest, second-nearest, and third-nearest neighbors on a three-dimensional cubic lattice of size $N = L^3$ with periodic boundaries. Each of the sites has connectivity $c = 26$, and a set of coupling constants $\mathcal{J} = \{J_{ij}\}$ consists of quenched random variables chosen from a bimodal distribution $P(J_{ij}) = x\delta(J_{ij} - J) + (1 - x)\delta(J_{ij} + J)$, where

x denotes the fraction of ferromagnetic couplings. To prevent a ferromagnetic transition, we set $x = (1 - 1/\sqrt{2})/2 \simeq 0.15$ and $J = \sqrt{2}J_0$. Then, the mean and variance of the couplings are -1 and 1, respectively, measured in units of J_0. This means that most of the couplings are antiferromagnetic in this model. Note that because all the spins in the smallest cube with $L = 2$ interact with each other through up to the third-nearest-neighbor couplings, a finite frustration remains for $p \leqslant 7$ even in the purely antiferromagnetic case. In this Rapid Communication, we focus on the case of $p = 7$.

Since spin-glass simulations are hampered by extremely slow relaxation dynamics, we use the replica exchange Monte Carlo method [22]. The linear sizes are $L = 4$–10 for most of the observables explained below and $L = 14$ for the energy density and specific heat, which are relatively easy to evaluate. The number of samples averaged over is 256–4096 depending on the system size. The total number of Monte Carlo sweeps (MCS) used on each lattice size is 10^6–10^8. We examined equilibration by monitoring the Monte Carlo average of the observables while doubling the number of MCS for successive measurements. The data are regarded as equilibrium values when the last two data agree within their error bars.

Observables. It is convenient to represent the Potts variables using the simplex representation [23], in which the spin variable $\boldsymbol{S}_i$ of site i takes one of p unit vectors $\{\boldsymbol{e}^{(\alpha)}\}_{\alpha=1}^{p}$ pointing to the corner of the simplex in $(p-1)$-dimensional space. These vectors satisfy the relations $\boldsymbol{e}^{(\alpha)} \cdot \boldsymbol{e}^{(\beta)} = (p\delta_{\alpha,\beta} - 1)/(p-1)$. Some observables calculated in our simulations are expressed as those in vector spin glasses using the simplex representation. To study the spin-glass transition, we define a spin-glass order parameter as an overlap between two replicas. For two independent replica configurations, denoted as $\{\boldsymbol{S}_i^{(1)}\}_{i=1}^{N}$ and $\{\boldsymbol{S}_i^{(2)}\}_{i=1}^{N}$ with the same disorder, the wave-number-dependent overlap between them for the Potts glass model is defined by the tensor $q^{ab}(\boldsymbol{k})$:

$$q^{ab}(\boldsymbol{k}) = \frac{1}{N}\sum_{i=1}^{N} S_i^{a,(1)} S_i^{b,(2)} e^{i\boldsymbol{k}\cdot\boldsymbol{R}_i}, \quad (2)$$

where the superscripts a and b are indices of the simplex vector component, and $\boldsymbol{R}_i$ is a displacement vector at site i. A rotational invariant scalar overlap is also defined as

$$q(\boldsymbol{k}) = \sqrt{\sum_{a,b}^{p-1} |q^{ab}(\boldsymbol{k})|^2}. \quad (3)$$

Then, the wave-number-dependent spin-glass susceptibility $\chi_{\rm SG}(\boldsymbol{k})$ is given by an expectation value

$$\chi_{\rm SG}(\boldsymbol{k}) = N[\langle q^2(\boldsymbol{k})\rangle^{(T)}]_{\rm av}, \quad (4)$$

where $[\cdots]_{\rm av}$ and $\langle\cdots\rangle^{(T)}$ represent an average over the quenched disorder and a thermal average at temperature T, respectively. The dimensionless correlation length ξ_L/L is useful for estimating the critical temperature T_c because it is independent of L at T_c. Thus, the intersection temperature in the plot of ξ_L/L for various L values gives an estimate of T_c. The finite-size correlation length ξ_L is estimated from $\chi_{\rm SG}(\boldsymbol{k})$ as [24]

$$\xi_L = \frac{1}{2\sin(|\boldsymbol{k}_{\min}|/2)}\sqrt{\frac{\chi_{\rm SG}(\boldsymbol{0})}{\chi_{\rm SG}(\boldsymbol{k}_{\min})} - 1}, \quad (5)$$

where $\boldsymbol{k}_{\min} = (2\pi/L, 0, 0)$ is the smallest nonzero wave vector. Another dimensionless quantity is the Binder parameter, which is defined as

$$g_4 = \frac{(p-1)^2}{2}\left(1 + \frac{2}{(p-1)^2} - \frac{[\langle q^4(\boldsymbol{0})\rangle^{(T)}]_{\rm av}}{[\langle q^2(\boldsymbol{0})\rangle^{(T)}]_{\rm av}^2}\right). \quad (6)$$

This quantity is known to exhibit peculiar behavior for systems with a one-step replica symmetry breaking (1RSB) transition [25–27], while it is expected to exhibit intersection at a conventional second-order transition temperature.

One of the most important quantities for studying the phase space structure of the spin-glass phase is the overlap distribution function

$$P^{(T)}(Q) = [\langle\delta[Q - q(\boldsymbol{0})]\rangle^{(T)}]_{\rm av}, \quad (7)$$

which is accessible from Monte Carlo simulations. The overlap distribution function has a nontrivial structure if RSB occurs. In particular, two separate peaks appear in $P^{(T)}(Q)$ at and below T_c for a 1RSB system, which is similar to the order parameter distribution found in systems with a first-order transition.

Numerical results. First, to investigate the critical properties of the Potts glass model, we examine the finite-size correlation length ξ_L scaled by L. As shown in Fig. 1, a clear intersection is observed around $T/J \simeq 0.4$, though it shifts slightly to low temperature with increasing L. The intersection for an asymptotically large L provides evidence of a spin-glass phase transition at the temperature. The Potts glass model for $p = 7$ with nearest-neighbor interactions has no glassy phase down to very low temperature, possibly down to zero with the present fraction of ferromagnetic couplings. The second- and third-nearest-neighbor couplings increase the spin-glass transition temperature significantly. To determine T_c and ν, we perform a finite-size scaling analysis in which

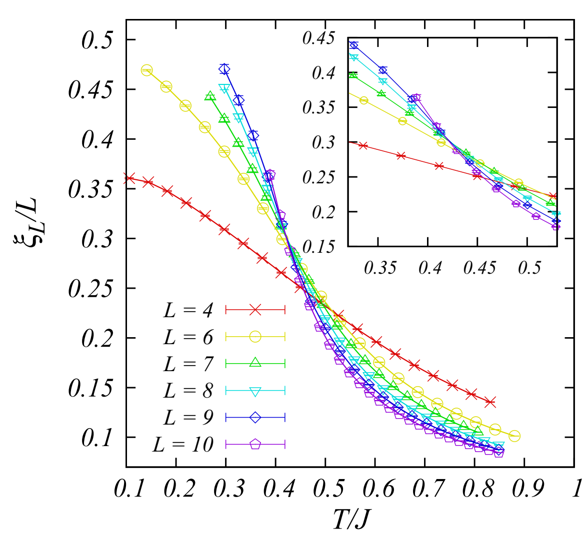

FIG. 1. (Color online) Temperature dependence of the dimensionless correlation length ξ_L/L. Inset shows enlarged view around the transition temperature.

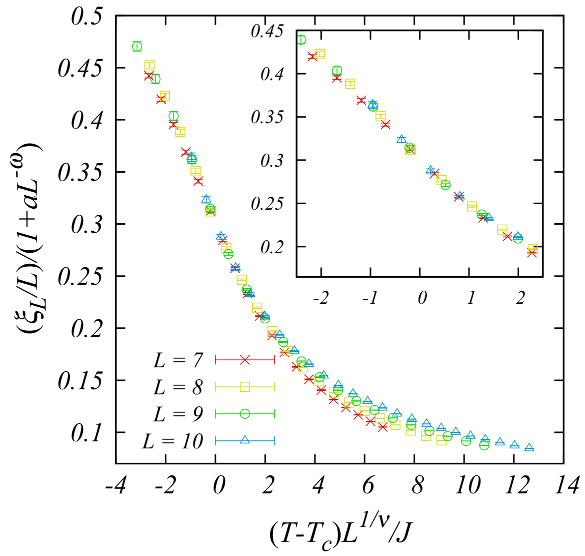

FIG. 2. (Color online) Scaling plot of the finite-size correlation length ratio ξ_L/L according to Eq. (8) using $T_c/J = 0.421$, $\nu = 0.68$, $a = 1$, and $\omega = 3$. Inset shows magnified view.

the dimensionless correlation length is assumed to follow the scaling form up to the leading correction term,

$$\frac{\xi_L}{L} = \widetilde{X}[(T - T_c)L^{1/\nu}](1 + aL^{-\omega}), \tag{8}$$

where ν is the correlation length exponent, ω is an exponent of the leading correction, and $\widetilde{X}$ is a universal scaling function. The scaling parameters such as T_c and ν are determined by requiring all the curves of $\xi_L/[L(1 + aL^{-\omega})]$ against $(T - T_c)L^{1/\nu}$ to collapse on a single curve near T_c. A recently developed Bayesian scaling analysis [28] is used to perform the scaling analysis systematically. Figure 2 shows the scaling plot of ξ_L/L, which is obtained by

$$T_c/J = 0.421(3), \quad \nu = 0.68(9). \tag{9}$$

The value of ν is consistent with $2/d$, where d is the spatial dimension, which was derived by a heuristic scaling argument based on the RFOT [29], suggesting that the overlap function has a finite jump at T_c. This is in contrast with the fact that the value of ν is slightly larger than $2/d$ in three-dimensional Potts glass models with the nearest-neighbor couplings [15–17].

Figure 3 shows the temperature and system-size dependence of $P^{(T)}(Q)$. At high temperatures, the distribution function has a single Gaussian-like peak near $Q \simeq 0$. The peak position is expected to approach zero in the thermodynamic limit. On the other hand, below T_c another peak at a larger value of Q, corresponding to the Edwards-Anderson order parameter $q_{\rm EA}$, emerges and coexists with the other peak at lower Q. The lower panel in Fig. 3 shows the size dependence of $P^{(T)}(Q)$ at $T/J = 0.2970$, which is well below the estimated T_c. The peaks at $Q = q_{\rm EA}$ and $Q \simeq 0$ tend to grow in height and become narrower with increasing L. Further, the weight between these two peaks is strongly suppressed with L. These behaviors imply that the bimodal structure in $P^{(T)}(Q)$ remains in the thermodynamic limit, providing clear evidence of the 1RSB nature of the spin-glass phase.

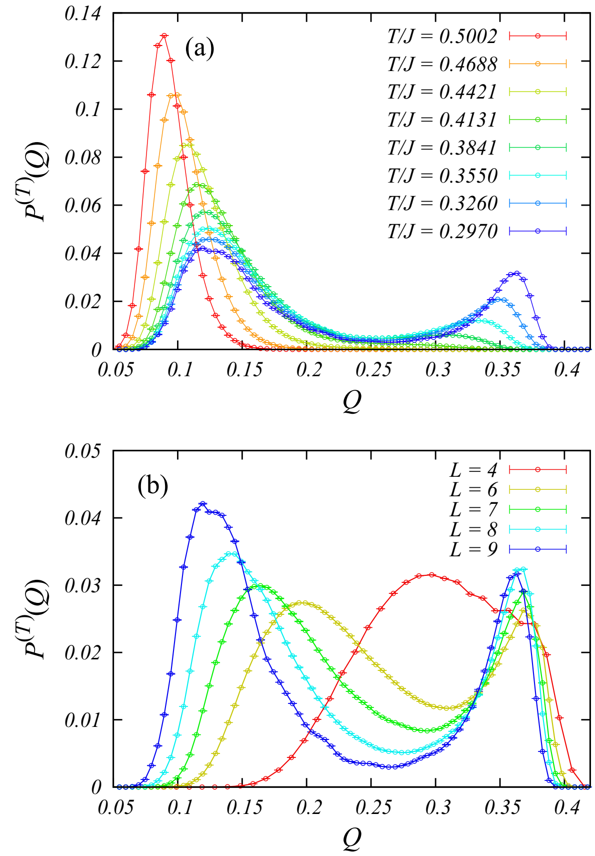

FIG. 3. (Color online) Overlap distribution function of a Potts glass model in three dimensions (a) for various temperatures with $L = 9$ and (b) for different sizes at $T/J = 0.2970$ below T_c.

While Fig. 3(a) suggests that the overlap emerges discontinuously at T_c, the peak of $P^{(T)}(Q)$ near T_c is rounded by the finite-size effect. Additional evidence of the discontinuous jump is found, however, in the temperature dependence of the Binder parameter g_4. As shown in Fig. 4, g_4 exhibits a negative dip near T_c with a negatively divergent tendency for large L. Note that $g_4 \to -\infty$ at T_c when a 1RSB transition with a finite jump of $q_{\rm EA}$ occurs in the mean-field glass models [25,27], in contrast to a continuous full RSB transition and also

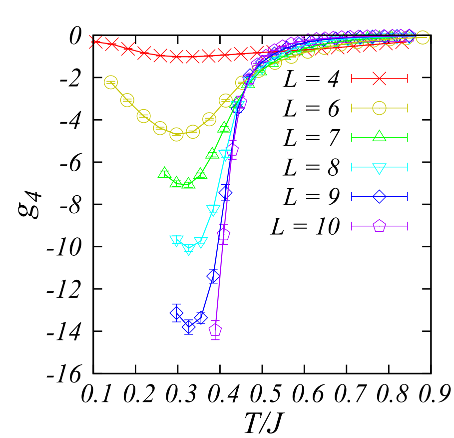

FIG. 4. (Color online) Temperature dependence of the Binder parameter g_4 of a Potts glass model in three dimensions.

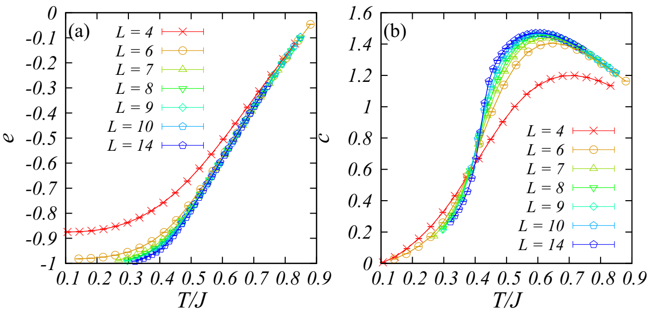

FIG. 5. (Color online) Temperature dependence of (a) energy density and (b) specific heat.

an ordinary second-order phase transition. Thus, this divergent behavior implies that q_{EA} appears discontinuously at T_c.

Finally, Fig. 5 shows the temperature dependence of the energy density and specific heat. No discontinuity in the energy density, and hence no divergent tendency in the specific heat, are observed at around T_c. Instead, the specific heat for various sizes has an intersection near T_c. This might indicate that in the thermodynamic limit the specific heat has a discontinuous jump at T_c, as expected from some mean-field spin-glass models with the RFOT. Further study is required to clarify this point.

Conclusions. In this Rapid Communication, the seven-state Potts glass model with the nearest-, second-nearest-, and third-nearest-neighbor interactions was proposed as a candidate for displaying the RFOT in finite dimensions. A key aspect is the maintenance of both a large number of Potts states and frustration. All of our equilibrium numerical results suggest that the present model in three dimensions shares many features of the RFOT, namely, a spin-glass transition at finite temperature, a jump in the spin-glass order parameter at T_c without latent heat, and a bimodal overlap distribution below T_c, as expected from 1RSB. Thus, we conclude that this is a realization of a finite-dimensional statistical-mechanical model that mimics the static part of the entire RFOT scenario. Another important aspect of the RFOT scenario is its dynamical properties, which are believed to be modified in finite dimensions from the mean-field predictions. This model provides a promising test bed for further examining the validity of the RFOT scenario in finite dimensions, which remains to be investigated.

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