Low-temperature properties of the $\pm J$ Ising spin glass in two dimensions

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The replica Monte Carlo simulation method and finite-size transfer-matrix method are used to study low-temperature properties of the $\pm J$ Ising spin glass in two dimensions. We find the spin-glass susceptibility exponent $\gamma = 5.11 \pm 0.05$ with a zero-temperature transition. The ground-state entropy $s_0 = 0.071 \pm 0.007$ by Monte Carlo simulation agrees well with previous transfer-matrix calculation, and the specific heat at low temperature has an asymptotic form $c/k_B \approx 1.3 J^2/(k_B T)^2 e^{-2J/(k_B T)}$, which indicates an energy $2J$ as low-lying excitations. We show that the replica Monte Carlo method is much faster than standard annealing for finding ground states.

I. INTRODUCTION

The spin-glass problem has been an interesting and difficult problem.[1,2] Recent large-scale computer simulations for short-range models give strong evidence of a finite-temperature transition from a paramagnetic phase to a spin-glass phase in three dimensions.[3,4] However, the low-temperature spin-glass phase is still not very well understood.[5,6] In two dimensions, a phase transition occurs only at zero temperature.[7-9] In this paper we concern ourselves with the two-dimensional model at low temperatures. Using a recently proposed new Monte Carlo simulation technique, replica Monte Carlo method,[9] we can equilibrate the system at much lower temperature than previously possible by the standard Monte Carlo method. The new method gives the spin-glass susceptibility exponent $\gamma = 5.11 \pm 0.05$ in agreement with a high-temperature expansion result.[10] The zero-temperature entropy s_0, from integrating specific-heat data, is in good agreement with transfer-matrix results,[11] while previous Monte Carlo work gave a larger value.[12] We also find a peculiar property of the asymptotic low-temperature specific heat $c/K^2 \approx 1.3 e^{-aK}$ ($K = J/k_B T$). The "elementary excitation" for the system is $a = 2$ instead of 4, which might be naively expected.

In the next section, the spin-glass model and the replica Monte Carlo method are described. A study of the replica Monte Carlo method for finding ground states is given in Sec. III. The replica Monte Carlo method is shown to give fast annealing speed to a ground state. The susceptibility and correlation length data are discussed in Sec. IV, and energy, specific heat, and entropy calculations are presented in Sec. V. A summary is given in the last section.

II. REPLICA MONTE CARLO METHOD

The Monte Carlo method[13] is a way of sampling the states in configuration space according to a desired Gibbs distribution by a Markov process. A difficulty, which becomes severe near a phase transition, is that the states so generated are highly correlated (critical slowing down). Although the long-time correlation has physical significance,[14] it severely hampers the application of the method. The replica Monte Carlo method[9] is aimed at reducing correlations in spin-glass simulations. The correlation time of the replica Monte Carlo algorithm has been reported in Ref. 9. Here we give a description of the algorithm. In the next section the efficiency of ground-state search by replica Monte Carlo method will be presented.

Consider an Ising spin glass, defined by the Hamiltonian[15]

$$H = K \sum_{\langle i,j \rangle} B_{ij} \sigma_i \sigma_j \ , \tag{1}$$

where σ_i takes on the values ± 1 and the factor $-J/k_B T$ has been absorbed into the coupling constant K. The B_{ij} are dimensionless variables, which describe the quenched, random interactions. In this study, we take the independent, equally probable $+1$ or -1 distribution. The interactions are nearest neighbor only.

Instead of simulating different temperatures sequentially, n replicas of the system are simulated simultaneously. Each of them obeys the same Hamiltonian (the same set of coupling), but is in different states and at different temperatures. The Hamiltonian for the whole system is

$$H_{\rm rep}(\sigma) = \sum_{a=1}^{n} H^a(\sigma^a) = \sum_{a=1}^{n} K^a \sum_{\langle i,j \rangle} B_{ij} \sigma_i^a \sigma_j^a \ . \tag{2}$$

If we simulate $H_{\rm rep}(\sigma)$ by standard Monte Carlo method, the system is just n independent original spin-glass systems. An important point is to pass "information" between replicas. Consider two replicas, a and b. The Hamiltonian for the pair is

$$H_{\rm pair}(\sigma) = \sum_{\langle i,j \rangle} B_{ij} (K^a \sigma_i^a \sigma_j^a + K^b \sigma_i^b \sigma_j^b) \ . \tag{3}$$

Introduce new variables, $\tau_i^{ab} = \sigma_i^a \sigma_i^b$, which are closely related to the spin-glass order parameter q. If two replicas are at the same temperature, then $q = [\langle \tau_i^{ab} \rangle]_B$, where angular brackets indicate the thermodynamic average and square brackets indicate the average over random couplings. The spins τ_i^{ab} form clusters or domains of $+$ spins and $-$ spins. They give more information of the spin-glass ordering than the original variables. Within

each cluster the σ spins of two replicas change their directions in a coherent fashion. When crossing boundaries of the clusters this coherent property is lost. Thus τ_i^{ab} spins are important variables. We eliminate one of the original spin-glass variables σ_i^b in favor of τ_i^{ab}. Using $\sigma_i^b/\sigma_i^a=\sigma_i^b\sigma_i^a=\tau_i^{ab}$ (since $\sigma^2=1$), Eq. (3) is rewritten as

$$H_{\text{pair}}(\sigma)=\sum_{\langle i,j\rangle} B_{ij}\sigma_i^a\sigma_j^a(K^a+K^b\tau_i^{ab}\tau_j^{ab}) . \quad (4)$$

Holding τ_i^{ab} fixed, we observe that the couplings are strengthened in the region of τ clusters. In those regions, the coupling is proportional to K^a+K^b, roughly twice of the original couplings if K^a and K^b are close. This tends to make the σ spins strongly locked and form rigid clusters. On boundaries of τ clusters, couplings are proportional to K^a-K^b. So the couplings between clusters are much weaker, all σ spins within a cluster can then be turned over with little cost of energy. In a standard single-spin-flip Monte Carlo simulation, the domain structure is not used. To flip a whole cluster takes a long time.

In replica Monte Carlo method, the τ clusters are used as a template, a usual Monte Carlo method on the *clusters* is performed. This is equivalent to simulating an effective Hamiltonian for the clusters during one Monte Carlo updating,

$$H_{\text{cl}}(\eta)=\sum_{(\alpha,\beta)} k_{\text{eff}}^{\alpha\beta}\eta_\alpha\eta_\beta \quad (5)$$

with the interactions between clusters given by

$$k_{\text{eff}}^{\alpha\beta}=\sum_{\alpha,\beta\ \text{boundary}} B_{ij}\sigma_i^a\sigma_j^a(K^a-K^b) , \quad (6)$$

where the summation is carried over the boundary between clusters α and β. σ_i^a is the value before updating. Each cluster α is associated with a new Ising variable η_α, initialized to $+1$. After updating each cluster, new states are obtained through $\sigma_i'^a=\sigma_i^a\eta_\alpha$, $\sigma_i'^b=\sigma_i^b\eta_\alpha$ for site i belongs to cluster α. The τ spins are fixed during one Monte Carlo updating. This is necessary in order to maintain the cluster configuration unchanged.

Replicas are arranged at successive temperatures separated by a constant $\Delta K=K^a-K^b$. Each replica interacts with its neighbor replicas through the above described algorithm. We do not let $\Delta K=0$. Although that leads to cluster flip without cost of energy, what it does is only an exchange of configurations between two replicas. The parameter ΔK and the number of replicas n can be adjusted to minimize correlation. The number of replicas are essentially limited by computer memory and speed. We like to have a whole range of temperatures. So ΔK is chosen by considering these two factors.

The above simulating process alone does not lead to transitions from any configuration to any other configuration. Certain transitions are forbidden. As an example, suppose all spins are in up state, $\sigma_i^a=+1$, as the algorithm is applied, the system always stays in all spin-up or all spin-down state. To ensure ergodicity, a standard Monte Carlo simulation on the original spin-glass system is used. The whole combined process obeys detailed balance and correctly generates the states of the original Hamiltonian.

Replica Monte Carlo techniques can also be combined with the Potts percolation algorithm.[16] When the Potts-percolation transformations are applied only to the interactions inside τ clusters, it further breaks the clusters and ergodicity is ensured without invoking standard Monte Carlo.

III. GROUND STATES

The replica Monte Carlo simulation method is applied to the problem of a ground-state search by annealing. It is compared with a standard Monte Carlo method. The problem has its applications in optimization subject to conflicting constraints.[17]

To make sure a ground state is actually obtained, an independent method to calculate the ground-state energy for given set of random interactions is necessary. There are exact polynomial-time algorithms for the two-dimensional problem.[18–20] The algorithm of Lawler[19] executes in a time of order L^6, here L is the linear size of a two-dimensional lattice. The algorithm is complicated and the dependence of computer time with size is still strong in practice. A second method is Morgenstern and Binder's exact transfer-matrix calculation of the partition function.[7] Summation of spins is performed row by row. This reduces the number of operation from 2^{ML} of a naive enumeration of all the states to $ML2^L$ for a $M\times L$ stripe. One data point for a 12×12 lattice takes 40 s on a MicroVax II, which is fast enough to allow us to determine the ground-state entropy, the ground-state energy, and the first-excited-state degeneracy. We fit the reduced free energy, with free boundary conditions for a given set of random couplings, to a form

$$f=\frac{1}{N}\ln Z=s_0-e_0K+\frac{g_2}{Ng_0}\exp(-aK)+\cdots , \quad (7)$$

where g_0 and g_2 are the degeneracy of ground states and first excited states. The zero-temperature entropy is given by $s_0=(\ln g_0)/N$. The ground-state energy per spin e_0 can be obtained to high accuracy.

We simulated the two-dimensional Ising spin-glass model with 16 replicas. The dimensionless inverse temperatures K are set at various values from 0.4 to 10 or 20. This differs from the usual annealing, since we do not vary the temperature of each replica. For the largest K, system is essentially at zero temperature. Table I is a list of typical time in Monte Carlo steps to reach a ground state, starting from random configurations. The standard

TABLE I. Monte Carlo steps needed to reach ground states of the two-dimensional ±J Ising spin-glass model by replica Monte Carlo with 16 replicas and by standard Monte Carlo from Ref. 7.

Size L	Replica MC	Standard MC
8	5–20	10^3–10^4
12	10–40	3×10^4
18	20–200	3×10^4–6×10^4
24	40–200	8×10^4
32	60–600	1×10^5–2×10^5

Monte Carlo data from Morgenstern and Binder[7] are also listed for comparison. The time to reach a ground state depends on the size of the system, and also depends on the starting configurations and random couplings. Those runs of sizes $L \leq 12$ are checked against exact values. Results of larger sizes are compared between several runs. The replica Monte Carlo is 100 to 1000 times faster in terms of Monte Carlo steps per spin. If we take into account of the fact that 16 replicas are simulated simultaneously, we still gain roughly a factor of 10 or more.

The ground-state energy per spin, extrapolated to infinite lattice size based on data from 8×8 to 32×32 lattices, is $e_0=-1.407\pm0.008$. This is in good agreement with transfer-matrix calculation of Morgenstern and Binder.[7] The latest transfer-matrix result of Cheung and McMillan[11] is $e_0=-1.4024\pm0.0012$.

IV. SUSCEPTIBILITY AND CORRELATION LENGTH

The spin-glass susceptibility, defined by

$$\chi_{\rm SG}=\frac{1}{N}\sum_{i,j=1}^{N}[\langle\sigma_i\sigma_j\rangle^2]_B =\frac{1}{N}\left[\left\langle\left[\sum_{i=1}^{N}\tau_i\right]^2\right\rangle\right]_B , \tag{8}$$

is calculated on a 128×128 lattice. Two sets of replicas with the same distribution of temperatures are used in order to obtain $\tau_i=\sigma_i^1\sigma_i^2$. Figure 1 shows $\chi_{\rm SG}$ versus K in a log-log scale. The data are averages of two to eight runs, depending on data points. The largest coupling for which McMillan[8] obtained reliable data by the standard Monte Carlo was $K=1.16$ ($\log_{10}K=0.06$). The data lay fairly well on a straight line for $\log_{10}K>0.1$, indicating a power-law behavior with a zero transition temperature. We use a least-squares fit of the form $\chi_{\rm SG}=aK^{\gamma}$. The fitting results in an exponent $\gamma=5.11\pm0.05$. This is larger than found in the previous work.[8,21] It is in agreement with a recent high-temperature series result $\gamma=5.3\pm0.3$ by Singh and Chakravarty.[10]

The spin-glass spatial correlation function,

$$g_{\rm SG}(r)=\frac{1}{N}\sum_{i=1}^{N}\langle\sigma_i\sigma_{i+r}\rangle^2=\frac{1}{N}\sum_{i=1}^{N}\langle\tau_i\tau_{i+r}\rangle , \tag{9}$$

is calculated on a 128×128 lattice. It is least-square fitted to

$$g_{\rm SG}(r)=A\frac{\exp(-r/\xi)}{r^{\eta}} . \tag{10}$$

The fit gives a constant $A=0.77\pm0.02$ for $K=0.6$–8.0. Figure 2 is a plot of the correlation length ξ versus K in a log-log scale. A power-law divergence $\xi\sim K^{\nu}$ is expected. An exponent $\nu=2.8\pm0.2$ gives the best fit to the data. This value is slightly larger than McMillan's result $\nu=2.64\pm0.38$ (Ref. 8) obtained in the range $K=0.667$–1.16. As we can see from the plot, one would get a smaller slope at smaller couplings. The exponent η in the fitting has a temperature dependence. It is $\eta=0.33$–0.28 in the coupling range $k=1.2$–2.6. At stronger couplings, η decreases to 0.25–0.22. From the scaling relation $\gamma=\nu(2-\eta)$, using $\gamma=5.11\pm0.05$ and $\nu=2.8\pm0.2$, we obtain $\eta=0.18\pm0.15$. The error is large, mainly due to uncertainty of ν, and it is smaller

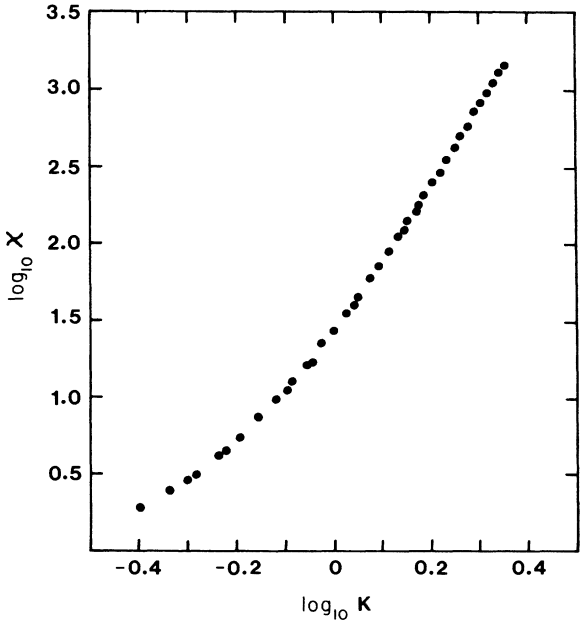

FIG. 1. Log-log plot of the spin-glass susceptibility as a function of the dimensionless inverse temperature K for the two-dimensional $\pm J$ Ising spin-glass on a 128×128 lattice, with use of several random interaction distributions with up to 1.8×10^4 Monte Carlo steps per site.

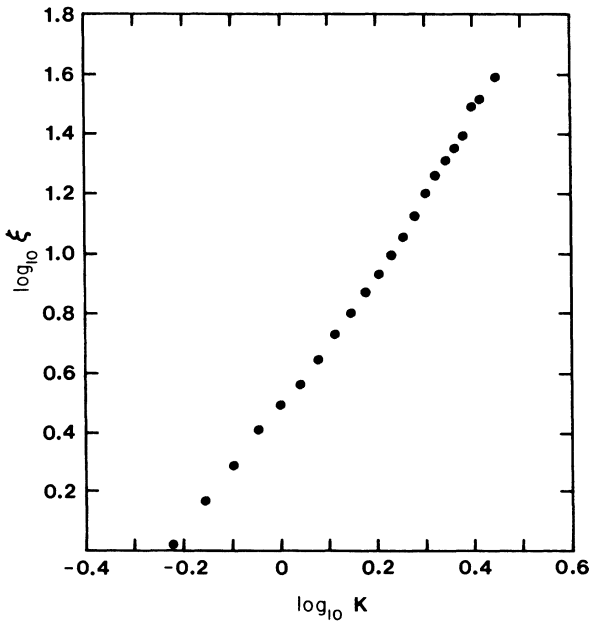

FIG. 2. Log-log plot of the correlation length ξ vs the coupling K for the two-dimensional $\pm J$ Ising spin-glass model.

than the value obtained by direct fitting. However, in the direct three-parameter fitting, the value η does go to a smaller number at large couplings. We think that a more accurate estimate of the exponent η is given by a Monte Carlo renormalization group study,[22] $\eta=0.20$. This is in agreement with the scaling result 0.18 ± 0.15. McMillan[8] obtained the somewhat higher value of $\eta=0.28\pm0.04$.

V. ENERGY, SPECIFIC HEAT, AND ENTROPY

The replica Monte Carlo method provides accurate results of the energy and specific heat for spin glasses. Figure 3 is the energy e and the reduced specific heat c/K^2 per spin for the two-dimensional $\pm J$ Ising spin-glass model plotted against $1/K$. The smooth curves are high-temperature expansion results

$$e=-2x+4x^7-4x^9+\cdots , \tag{11}$$

$$\frac{c}{K^2}=-\frac{de}{dK}=(2-28x^6+36x^8)(1-x^2)+\cdots , \tag{12}$$

where $x=\tanh K$. These high-temperature expansions give a good description of the energy and specific heat up to $K\approx0.6$.

The specific-heat data are used to calculate the zero-temperature entropy by[12]

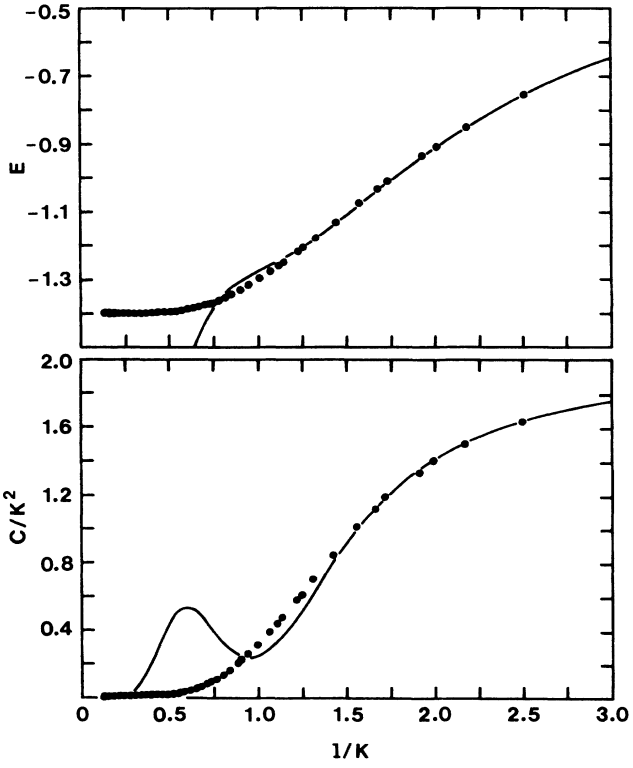

FIG. 3. The energy and the reduced specific heat vs the dimensionless temperature for the $\pm J$ Ising spin-glass model in two dimensions. Data are average of several runs on 64×64 lattice. The smooth curves are high-temperature expansion results.

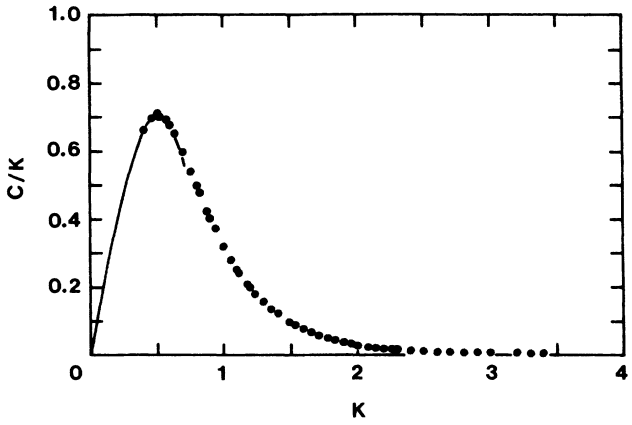

FIG. 4. The specific heat c over the dimensionless coupling K vs K of the two-dimensional $\pm J$ Ising spin-glass model. The smooth curve is the high-temperature expansion result. Data are averages of 4–17 runs on 64×64 and 128×128 lattices. The area under the curve is used to estimate the zero-temperature entropy.

$$s_0=\ln2-\int_0^\infty \frac{c}{K}dK . \tag{13}$$

Figure 4 is a plot of the integrand. On the high-temperature ($K<0.5$) part, Eq. (12) is used. We obtained $s_0=0.071\pm0.007$. This value is smaller than Kirkpatrick's[12] result of $s_0=0.99$ using a similar method by the standard Monte Carlo techniques. Our result is in good agreement with the transfer-matrix calculation of Morgenstern and Binder,[7] and also with estimates of Vannimenus and Toulouse.[23] The latest, most accurate (transfer-matrix) value of Cheung and McMillan[11] is $s_0=0.0701\pm0.0005$. A larger value from the previous Monte Carlo result was interpreted as a dynamic effect.

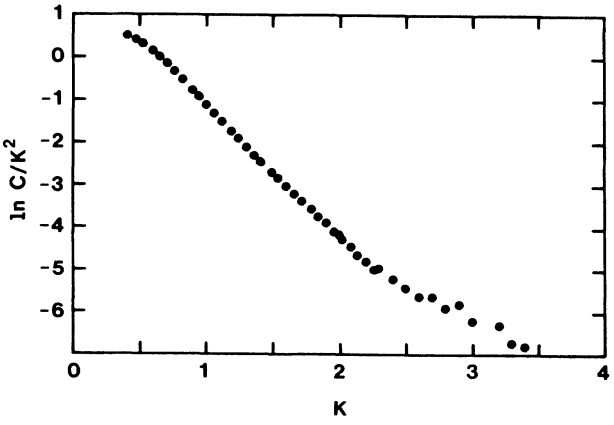

FIG. 5. Semilogarithmic plot of the reduced specific heat c/K^2 vs coupling K for the two-dimensional $\pm J$ Ising spin-glass model.

One of the interesting features of the specific heat is its low-temperature behavior. Figure 5 is a plot of c/K^2 versus K in a semilogarithmic scale. The reduced specific heat c/K^2 behaves like an exponential of the form $\exp(-3K)$ in a large range from $K=0.6$ to 2. Then it bends over to a slope close to -2. For a system with discrete energy levels, the specific heat goes to zero exponentially with K,

$$c/K^2 \approx c_0 \exp(-aK) , \tag{14}$$

where a is determined by the lowest possible excitation in the system, for example, the lowest excited states in a two-dimensional Ising model are due to single reversed spins, and lie $8J$ above the ground state. The "elementary" excitation of the $\pm J$ spin glass is more subtle. For a finite system with periodic boundary conditions, a single-spin-flip gives the lowest excitation $4J$. On the other hand, unlike the ferromagnetic Ising model, where the number of such lowest possible excitations is proportional to the size N of the system, the number of $4J$ excitation grows much faster than N in the $\pm J$ Ising spin glass.

The one-dimensional nearest-neighbor Ising model provides an example to show how this happens. Simple calculation shows that the specific heat goes as $\exp(-2K)$ in the thermodynamic limit. But a finite system with a periodic boundary condition can only have $4J$ excitations (a kink-antikink pair). However, there are of order N^2 such excitations, so it is not elementary. A single kink is the lowest excitation for an infinitely long Ising chain, or a finite system with free boundary. The number of such single kinks is N, so it contributes a finite value to the specific heat in the large-N limit. Analogous to the one-dimensional Ising model, if we use free boundary conditions, the spin glass does have $2J$ excitations. An example is when a single spin on the boundary is flipped. Such an excitation can be moved into the interior of the system by rearrangements of a larger number of spins. We made a numerical calculation of the specific heat in the low-temperature limit with free boundary conditions using the transfer-matrix method of Morgenstern and Binder.[7] The data are fit to the form Eq. (14). It is found that a is unambiguously 2. We are interested in whether the coefficient $c_0=4g_2/(Ng_0)$ decreases with the size of the system. The value varies from realization to realization of the random couplings, but we do not observe a systematic size dependence (1.36, 1.16, 1.38, 1.28 for linear size 4, 8, 12, and 16). The best estimate for the coefficient is $c_0 \approx 1.3$. In summary, we believe that $2J$ is the correct lowest excitation. It is a nonlocal effect involving rearrangements of a large number of spin orientations.

VI. SUMMARY

The replica Monte Carlo method is shown to give faster speed for a ground-state search, which could have practical applications. The algorithm is very efficient to calculate thermodynamic quantities at low temperatures. The spin-glass susceptibility shows an asymptotic power-law behavior. We found a previously unnoticed behavior of the low-temperature specific heat, which is due to larger degeneracy of lower-level states. The zero-temperature entropy is in agreement with static calculations. Thus the replica Monte Carlo method gives true equilibrium states at very low temperatures for the two-dimensional Ising spin glass.

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