

Temperature Chaos and Bond Chaos in Edwards-Anderson Ising Spin Glasses: Domain-Wall Free-Energy Measurements

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Domain-wall free energy δF , entropy δS , and the correlation function C_{temp} of δF are measured independently in the four-dimensional $\pm J$ Edwards-Anderson (EA) Ising spin glass. The stiffness exponent θ , the fractal dimension of domain walls d_s , and the chaos exponent ζ are extracted from the finite-size scaling analysis of δF , δS , and C_{temp} , respectively, well inside the spin-glass phase. The three exponents are confirmed to satisfy the scaling relation $\zeta = d_s/2 - \theta$ derived by the droplet theory within our numerical accuracy. We also study bond chaos induced by random variation of bonds, and find that the bond and temperature perturbations yield the universal chaos effects described by a common scaling function and the chaos exponent. These results strongly support the appropriateness of the droplet theory for the description of chaos effect in the EA Ising spin glasses.

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In randomly frustrated systems such as spin glasses, directed polymer in random media (DPRM), and vortex glasses, the equilibrium ordered state could be completely reorganized by an infinitesimally small change in environment [1–7]. This curious property called the chaos effect has attracted much attention since it was found in the 1980s. Especially chaos induced by temperature variation (temperature chaos) is now of great interest because of its potential relevance for rejuvenation caused by temperature variation [8]. However, the issue of temperature chaos still remains far from being resolved. In particular, concerning low-dimensional Edwards-Anderson (EA) Ising spin-glass models, the situation is very controversial because numerical studies done so far provide the evidence both for and against temperature chaos [5,7,9–11].

In the present work, we examine temperature chaos by numerical measurements of the domain-wall free energy δF , the difference in the free energy between the system with the periodic boundary condition (BC) and that with the antiperiodic BC. This δF relates to the effective coupling J_{eff} between the two boundary spins S_L and S_R (see Fig. 1) as $J_{\text{eff}} = -\delta F/2$ [12,13]. We find δF of each sample exhibits oscillations along the temperature axis providing direct evidence of the temperature chaos. Furthermore, we find from simultaneous observations of the domain-wall energy δE and so entropy δS that δE and $T\delta S$ are large but they cancel with each other in the leading order to yield significantly small $\delta F = \delta E - T\delta S$. Such intriguing behavior is indeed predicted by the droplet theory [14]. For a quantitative check of the droplet theory we focus on the anticipated scaling relation

$$\zeta = d_s/2 - \theta \quad (1)$$

derived from it, where the stiffness exponent θ is extracted

from $\sigma_F \sim L^\theta$, the fractal dimension of domain walls from $\sigma_S \sim L^{d_s}$, and the so-called chaos exponent ζ from $C_{\text{temp}}(L, T, T + \Delta) \sim f[L(\Delta T)^{-1/\zeta}]$. Here σ_F and σ_S are the standard deviations of δF and δS , respectively, C_{temp} is the correlation function of δF 's defined by Eq. (4) below, and $f(x)$ is a certain scaling function. We find the three fundamental exponents thus extracted indeed satisfy Eq. (1) well inside the spin-glass phase whose thermodynamic properties are dominantly governed by the $T = 0$ fixed point.

We also study bond chaos by measuring how δF varies with changes in couplings. The result evidently shows the existence of bond chaos. Moreover, the scaling analysis of two correlation functions associated with temperature and bond perturbations reveals quantitatively that not only the chaos exponent but also the scaling function are common to both the perturbations. This universal aspect of chaos effect anticipated from the droplet theory [14] is also observed in the Migdal-Kadanoff spin glasses [15,16] and the DPRM [6]. All of our numerical results, particularly the quantitative check of Eq. (1), are strong evidence not only for the existence of chaos in the EA Ising spin glasses but also for the appropriateness of the droplet theory for its description.

The boundary flip MC method.—Let us first describe the boundary flip Monte Carlo (MC) method [17,18] which enables us to measure the domain-wall free energy. We

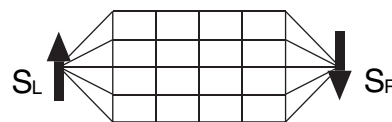


FIG. 1. Model for the boundary flip MC.

consider a model which consists of Ising spins on a d -dimensional hyper-cubic lattice of L^d and two *boundary* Ising spins S_L and S_R (see Fig. 1). The usual periodic BC is applied for the directions along which the two boundary spins do not lie. The Hamiltonian is $\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} S_i S_j$, where the sum is over all the nearest neighbor pairs including those consisting of one of the two boundary spins and a spin on the surfaces of the lattice. In our boundary flip MC simulation, the two boundary spins are also updated according to a standard MC procedure. For each spin configuration simulated, we regard the BC as periodic (antiperiodic) when S_L and S_R are in parallel (antiparallel). Since the probability $P_{P(AP)}(T)$ for finding the periodic (antiperiodic) BC is proportional to $\exp[-F_{P(AP)}(T)/T]$, where $F_{P(AP)}(T)$ is the free energy with the periodic (antiperiodic) BC, we obtain, with $P_{AP} = 1 - P_P$,

$$\begin{aligned} \delta F(T) &\equiv F_P(T) - F_{AP}(T) \\ &= -k_B T \{\log[P_P(T)] - \log[1 - P_P(T)]\}. \end{aligned} \quad (2)$$

We also measure the thermally averaged energy $E_{P(AP)}(T)$ when the two boundary spins are in parallel (antiparallel). It enables us to estimate the domain-wall *energy* $\delta E(T) \equiv E_P(T) - E_{AP}(T)$. Then, the domain-wall *entropy* δS is evaluated either from $\delta S = (\delta E - \delta F)/T$ or $\delta S = -\frac{\partial(\delta F)}{\partial T}$. We have checked that both the estimations yield identical results within our numerical accuracy.

We study the four-dimensional $\pm J$ Ising spin glasses in the present work. In four dimensions the value of the stiffness exponent θ is significantly large [18,19], which enables us to make scaling analyses rather easily as compared in three dimensions. The values of $\{J_{ij}\}$ are taken from a bimodal distribution with equal weights at $J_{ij} = \pm J$. We use the exchange MC method [20] to accelerate the equilibration. The temperature range we investigate is between $0.6J$ and $4.5J$, whereas the critical temperature of the model is around $2.0J$ [21]. The sizes we study are $L = 4, 5, 6, 7, 8, \text{ and } 10$. The number of samples is 824 for $L = 10$ and 1500 for the others. The period for thermalization and that for measurement are set sufficiently (at least 5 times) larger than the ergodic time, which is defined by the average MC step for a specific replica to move from the lowest to the highest temperature and return to the lowest one.

Temperature chaos.—In Fig. 2, we show temperature dependence of δF , δE , and $T\delta S$ for 5 samples. Oscillations of the three observables become stronger with increasing L . We, in fact, see that δF of some samples changes its sign, meaning that the favorable BC with the lower free energy changes with temperature. We also see that, as predicted by the droplet theory [14], $\delta E(T)$ and $T\delta S(T)$ exhibit very similar temperature dependence and cancel each other in the leading order to yield relatively small δF .

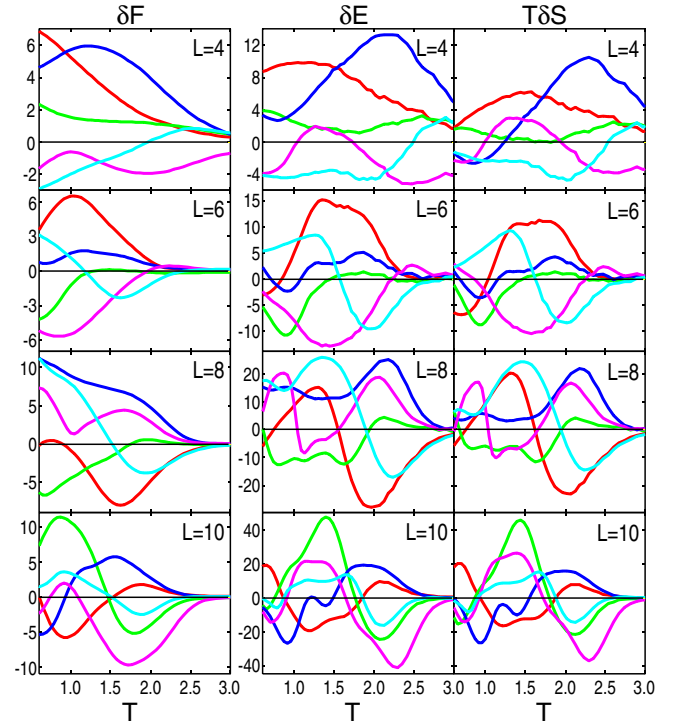


FIG. 2 (color online). δF (left), δE (middle), and $T\delta S$ (right) vs temperature for 5 samples. $L = 4, 6, 8, \text{ and } 10$ from top to bottom.

In Fig. 3, the standard deviations, σ_F , σ_E , and σ_S , at $T = 0.6J$ are plotted as a function of L . Interestingly, σ_S , which gives the amplitude of $|\frac{\partial(\delta F)}{\partial T}|$, increases more rapidly than σ_F , i.e., the amplitude of δF . See Ref. [11] for a similar observation in the three-dimensional EA model. As argued by Banavar and Bray [15], this result naturally leads

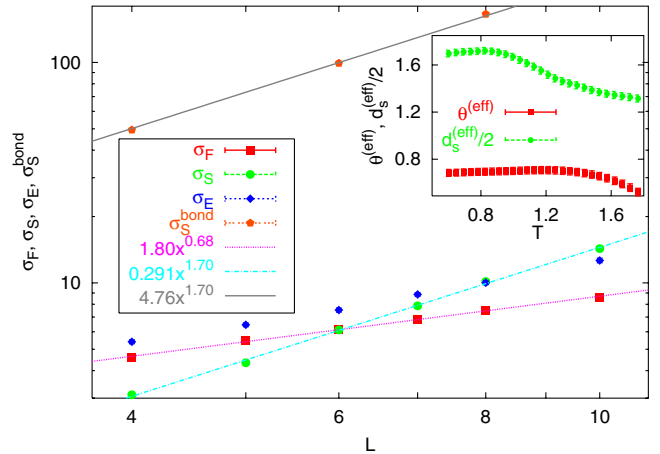


FIG. 3 (color online). Size dependences of σ_F , σ_E , σ_S , and σ_S^{bond} at $T = 0.6J$. See text for their definitions. The two straight lines for σ_F and σ_S are obtained by linear least-square fits of $\ln(\sigma_F)/\ln(\sigma_S)$ against $\ln(L)$. The line for σ_S^{bond} has the same slope as that for σ_S . The inset shows the data for $\theta^{(\text{eff})}$ and $d_s^{(\text{eff})}/2$.

us to the conclusion that δF in the limit $L \rightarrow \infty$ is totally temperature chaotic.

The inset of Fig. 3 shows $\theta(T)$ and $d_s(T)/2$ estimated by linear least-square fits of $\ln(\sigma_F)$ and $\ln(\sigma_S)$ against $\ln(L)$ at each temperature. As expected from the droplet theory which is constructed around the $T = 0$ fixed point, the two exponents converge to a certain value at low temperatures. By averaging over the lowest five temperatures, we obtain

$$\theta = 0.69 \pm 0.03, \quad d_s = 3.42 \pm 0.06. \quad (3)$$

Our θ is compatible with other estimations [18,19], while our d_s is somewhat smaller than other ones [22]. The apparent temperature dependence of $\theta(T)$ and $d_s(T)$ at higher temperatures is considered to be due to the critical fluctuation associated with the unstable fixed point at T_c , combined with the finite-size effect. Its detailed quantitative analysis is, however, beyond the scope of the present work.

We next examine the correlation function defined by

$$C_{\text{temp}}(L, T, T + \Delta T) \equiv \frac{\overline{\delta F(L, T) \delta F(L, T + \Delta T)}}{\sigma_F(L, T) \sigma_F(L, T + \Delta T)}, \quad (4)$$

where $\overline{\quad}$ is the sample average. A similar correlation function was first introduced by Bray and Moore to study bond chaos [4]. The inset of Fig. 4 shows the raw data of $1 - C_{\text{temp}}$ at $T = 0.6J$. C_{temp} approaches zero rapidly with increasing L . From the prediction of the overlap length by the droplet theory, over which the configurations at the two temperatures are unrelated, we expect one parameter scaling of $C_{\text{temp}} = f(L\Delta T^{1/\zeta})$ whose test is shown in the main frame of Fig. 4. We see that the scaling works nicely. The value of ζ is evaluated to be 1.12 ± 0.05 by the fitting. Quite interestingly, this value is consistent with the value

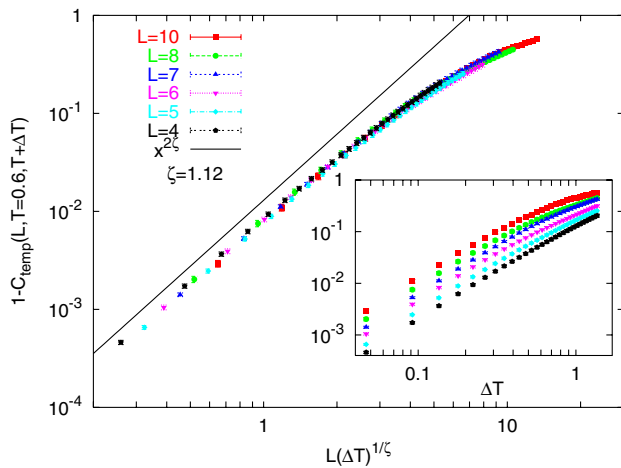


FIG. 4 (color online). A scaling plot of $1 - C_{\text{temp}}(L, T = 0.6, T = 0.6 + \Delta T)$ at $T = 0.6J$ against $L(\Delta T)^{1/\zeta}$ with $\zeta = 1.12$. The line is proportional to $x^{2\zeta}$. In the inset, $1 - C_{\text{temp}}$ for $L = 4, 5, 6, 7, 8,$ and 10 (from bottom to top) are plotted as a function of ΔT .

$\zeta = 1.02 \pm 0.06$ obtained by substituting Eq. (3) into Eq. (1) predicted by the droplet theory. This is one of the main results of the present work. We also see that the data are consistent with the expected asymptotic behavior in the limit $L^\zeta \Delta T \rightarrow 0$, $1 - C_{\text{temp}} \propto (L^\zeta \Delta T)^2$ [4], as depicted by the line.

Bond chaos and universality.—We also study bond chaos by comparing two systems with correlated coupling sets. The perturbed couplings $\{J'_{ij}\}$ are obtained from the unperturbed ones $\{J_{ij}\}$ by changing the sign of J_{ij} with probability p . Since simulation for bond chaos costs much more time than that for temperature chaos, we only examined $L = 4, 6, 8$ for bond chaos.

Now let us consider an observable $\delta S^{\text{bond}} \equiv -\frac{\delta F' - \delta F}{\Delta J}$, where $\Delta J \equiv \sqrt{p}$ and δF ($\delta F'$) is the domain-wall free energy of the unperturbed (perturbed) system. δS^{bond} here and δS discussed above are similar in a sense that the both are the increment ratios of δF against the perturbations. The ratio against ΔJ , not p itself, is considered to compare temperature perturbation and bond perturbation properly [5]. In Fig. 3, the standard deviation of δS^{bond} , denoted as σ_S^{bond} , is also shown. δS^{bond} is estimated with $\Delta J \approx 0.03$, which corresponds to a small value of $p \approx 0.0009$. The line for σ_S^{bond} and that for σ_S have the same slope, which suggests that temperature and bond perturbations belong to the same universality class. The coefficient of σ_S^{bond} is, however, about 16.4 times as large as that of σ_S . In the inset of Fig. 5 we show the raw data of the correlation function for bond perturbation defined by

$$C_{\text{bond}}(L, T, p) \equiv \frac{\overline{\delta F(L, T) \delta F'(L, T)}}{\sigma_F(L, T) \sigma_F'(L, T)}. \quad (5)$$

Again, the correlation decays faster with increasing L . In the main frame of Fig. 5, we test a similar scaling to that in

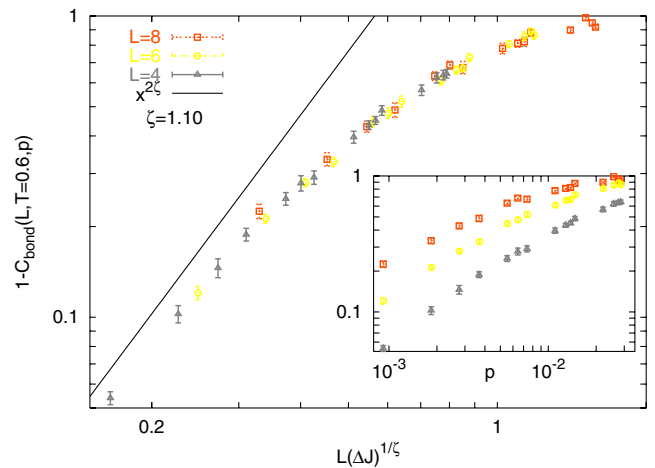


FIG. 5 (color online). A scaling plot of $1 - C_{\text{bond}}(L, T, p)$ at $T = 0.6J$ against $L(\Delta J)^{1/\zeta}$ with $\zeta = 1.10$, where $\Delta J = \sqrt{p}$. The line is proportional to $x^{2\zeta}$. In the inset, the raw data for $L = 4, 6,$ and 8 (from bottom to top) are shown as a function of p .

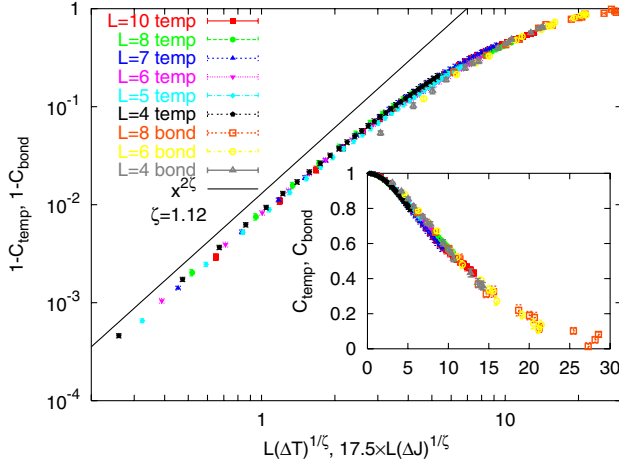


FIG. 6 (color online). A scaling plot of $1 - C$ by using all the data in Figs. 4 and 5. The scaling variable for the data of temperature perturbation is $L(\Delta T)^{1/\zeta}$, while that for the data of bond perturbation is $17.5 \times L(\Delta J)^{1/\zeta}$, where $\zeta = 1.12$. The line is proportional to $x^{2\zeta}$. The inset shows the same plot for C .

Fig. 4 by assuming that the overlap length of the bond perturbation scales as $\Delta J^{-1/\zeta}$. All the data again collapse into a single curve. The chaos exponent ζ is evaluated to be 1.10 ± 0.10 by the fitting.

To compare the two scaling functions for temperature and bond perturbations, we plot in Fig. 6 all the data of both C_{temp} and C_{bond} by using the same chaos exponent. Here we use the value $\zeta = 1.12$ in Fig. 4, and multiply the scaling variable $L(\Delta J)^{1/\zeta}$ by a factor of 17.5. All the data roughly merge into a single curve, indicating that the chaos exponent and the scaling function for temperature chaos are the same as those for bond chaos. Lastly, by estimating the overlap length ℓ as the value of L for which $C = 0.5$, we obtain

$$\ell_{\text{temp}} \approx 11.5 \Delta T^{-1/\zeta}, \quad \ell_{\text{bond}} \approx 0.657 \Delta J^{-1/\zeta}, \quad (6)$$

where $\zeta \approx 1.12$. We see that the overlap length of the bond perturbation is much shorter than that of the temperature one. This result, as well as the factor of 16.4 in the σ_S^{bond} scaling mentioned above, is the quantitative description of the well-known fact that temperature chaos is much more difficult to observe than bond chaos [5,11].

Conclusion.—In the present work, we have studied the four-dimensional EA Ising spin glass with a focus on the chaos effect. As a consequence, many nontrivial predictions of the droplet theory, such as the δF oscillation along the temperature axis and the cancellation of δE and $T\delta S$, are found in this model. Most importantly, the scaling relation of Eq. (1) and the universal aspect of temperature and bond chaos effects are quantitatively confirmed well inside its spin-glass phase whose thermodynamic properties are dominantly governed by the $T = 0$ fixed point.

These results are certainly strong evidences for the appropriateness of the droplet theory for the description of chaos effect in the EA Ising spin glasses. On the other hand, recent work by Rizzo and Crisanti [23] indicates the existence of similar chaos effects in the Sherrington-Kirkpatrick model. Whether our results are consistent with the mean field viewpoint or not is an interesting open problem.

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