Chaotic temperature and bond dependence of four-dimensional Gaussian spin glasses with partial thermal boundary conditions

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Spin glasses have competing interactions and complex energy landscapes that are highly-susceptible to perturbations, such as the temperature or the bonds. The thermal boundary condition technique is an effective and visual approach for characterizing chaos, and has been successfully applied to three dimensions. In this paper, we tailor the technique to partial thermal boundary conditions, where thermal boundary condition is applied in a subset (3 out of 4 in this work) of the dimensions for better flexibility and efficiency for a broad range of disordered systems. We use this method to study both temperature chaos and bond chaos of the four-dimensional Edwards-Anderson model with Gaussian disorder to low temperatures. We compare the two forms of chaos, with chaos of three dimensions, and also the four-dimensional ±J model. We observe that the two forms of chaos are characterized by the same set of scaling exponents, bond chaos is much stronger than temperature chaos, and the exponents are also compatible with the ±J model. Finally, we discuss the effects of chaos on the number of pure states in the thermal boundary condition ensemble.

I. INTRODUCTION

Chaos is a fascinating and common phenomenon in glassy systems, which have rugged energy landscapes such as spin glasses. The spin orderings are reorganized at large scales when a parameter is tuned, such as the temperature or the bonds. These corresponding chaotic phenomena are therefore called temperature chaos [1–16] and bond chaos [10, 11, 14, 17], respectively. While chaos is an equilibrium phenomena, it is also believed to be related to various non-equilibrium dynamics such as hysteresis, memory and rejuvenation effects [18–21]. Chaos is also of great relevance for numerical simulations and analog optimization machines [22, 23], such as the D-Wave quantum annealers. For example, small temperature perturbations or problem misspecifications could lead to a solution of an entirely different Hamiltonian, especially when the number of spins is large. Chaos is a source of the computational complexity of spin glasses [13, 15, 23, 24], known to slow down extended-ensemble algorithms, which are the current state-of-the-art methods, including both parallel tempering and population annealing. Therefore, chaos is closely related to both equilibrium and nonequilibrium properties of spin glasses, experimental optimizations, and numerical simulations.

It has been recognized that temperature chaos (TC) and bond chaos (BC) appear to follow the same scaling properties, and bond chaos is considerably stronger than temperature chaos [10, 11, 25]. Both of these results can be simply explained within the framework of the droplet picture [4, 26–29] by scaling properties and assuming that temperature chaos is mainly entropy driven, whereas bond chaos is mainly energy driven [17].

Most studies of chaos are based on some correlation functions [10, 11, 25, 30, 31]. Recently, a new technique called thermal boundary conditions (TBC) has been successfully applied to three-dimensional spin glasses [15, 17]. For thermal boundary conditions, the system can choose among periodic or antiperiodic boundary conditions in each spatial direction, according to the Boltzmann weights of the different boundary conditions. In D dimensions, the full TBC set has 2^D different boundary conditions. Chaos manifests itself as the instabilities of the relative weights of different boundary conditions (in thermal equilibrium) when the temperature or the bonds are tuned.

The TBC approach has certain advantages. Firstly, the strength of chaos is directly quantified using number of boundary condition crossings (exchange of their weights). Therefore, there is no reference state such as a reference temperature as in correlation functions. This allows a direct and detailed characterization of chaos such as the temperature dependence of the strength of temperature chaos. Chaotic events are also more frequently observed with the enlarged phase space, with some chaotic instances exhibiting several crossings in a typical parameter range (such as a temperature range for temperature chaos) even for a relatively small system size accessible to current simulations.

Despite of these successes and extensive research of chaos in three dimensions, there are far less work in four dimensions [6, 10, 31] and the majority of these work focus on the ±J model [6, 10]. To the best of our knowledge, we have only found one such pioneering numerical study on the Gaussian disorder in four dimensions operating at a relatively high temperature using correlation functions [31]. This is most likely due to earlier computational limitations, considering the Gaussian disorder is much harder to equilibrate than the ±J disorder. In this paper, we fill in this gap and study the numerically intensive four-dimensional Gaussian spin glasses to low temperatures (T_C/3 for temperature chaos and T_C/2 for bond chaos). This not only improves statistical errors.
for a better comparison of temperature chaos and bond chaos in 4D, but more importantly also allows us to compare with the 3D counterpart, and the 4D ±J model. Secondly, we also tailor the TBC technique to apply it more flexibly and efficiently to the 4D model (and many others, e.g., the one-dimensional chains with long-range interactions). Our work is done using partial thermal boundary conditions which is described as follows.

The motivation for the partial thermal boundary condition is from the following question: Is the total number of boundary conditions essential to the TBC technique? For example, is it necessary to keep all 16 boundary conditions in 4D, which is a rather expensive setup? Much computational efforts would be saved if we could reduce this number. On the other hand, for a one-dimensional spin chain with long-range interactions, one would like to use more boundary conditions rather than two to collect good statistics. In this work, we propose a simple idea to tailor the number of boundary conditions. More precisely, we introduce the partial thermal boundary conditions in four dimensions, to turn on thermal boundary conditions in only a subset of the dimensions. As mentioned, to collect good statistics, the number of boundary conditions should also not be too small. Therefore, we choose to keep 8 boundary conditions as in 3D, i.e., thermal boundary condition is turned on in three directions and periodic boundary condition is always applied in the fourth direction. Our results suggest that this method is valid, as shown in Sec. III.

The paper is organized as follows. We first present the model, simulation methods and scaling properties of temperature chaos and bond chaos in Sec. II, followed by numerical results in Sec. III. Concluding remarks are stated in Sec. IV.

II. MODELS AND NUMERICAL SETUP

In this Section, we present the four-dimensional Edwards-Anderson model, observables and simulation details. The scaling properties for characterizing the chaos phenomena are also summarized for completeness.

A. Models, methods and observables

The Edwards-Anderson (EA) Ising spin glass [32] is represented by the following Hamiltonian:

\[ H = - \sum_{\langle ij \rangle} J_{ij} S_i S_j, \]

where \( S_i \in \{\pm 1\} \) are Ising spins. The sum \( \langle ij \rangle \) is over the nearest neighbours in a four-dimensional simple cubic lattice of linear system size \( L \) and number of spins \( N = L^4 \). The couplings \( J_{ij} \) between spins \( S_i \) and \( S_j \) are chosen independently from the standard Gaussian distribution with mean zero and variance one. We refer to each disorder realization as an “instance”. We apply partial thermal boundary conditions (PTBC) to each instance, i.e., each instance has freedom to choose either periodic boundary conditions or antiperiodic boundary conditions in three directions according to the Boltzmann weights. In the fourth direction, periodic boundary condition is always applied. There are therefore a total of eight boundary conditions in our PTBC ensemble. More precisely, the weight \( p_i \) of a boundary condition \( i \) is related to its free energy \( F_i \) as:

\[ p_i = \frac{\exp(-\beta F_i)}{\sum_i \exp(-\beta F_i)}. \]

The model has a spin-glass phase transition at \( T_C \approx 1.8 \) [31, 33]. For later references, the 3D Gaussian model has \( T_C \approx 1 \) [34] and the 4D ±J model has instead \( T_C \approx 2 \) [35]. To study temperature chaos, a single instance \( J \) is cooled from the infinite temperature \( \beta = 0 \) to a low temperature deep in the spin-glass phase \( T_C/3 \). Scaling properties are studied in the temperature range \( T \in [T_C/3, 2T_C/3] \). To study bond chaos, we first choose an independent random perturbation instance \( J' \) for each instance \( J \). We then tune the bonds using a small parameter \( c \) at a fixed temperature \( T_C/2 \) following an annealing also from \( \beta = 0 \) as:

\[ J = J + c J', \]

where \( c \in [0, 0.1] \). The normalization factor is to preserve the standard Gaussian distribution for any \( c \) [11, 17, 25, 30, 31]. Note that the possibility to change the Gaussian bonds continuously over a range is a convenient advantage against discrete bonds such as the ±J model [10]. In our simulations, we start from \( c = 0.1 \) and then reduce \( c \) to 0, and the final instance becomes \( J \). Note that the final \( J \) is the identical temperature chaos instance for benchmarking purposes which will be used when we discuss thermal equilibration using that equilibrium properties should not depend on how the system is prepared. The simulations can be clearly visualized by looking at the simulation trajectories in the parameter space \((\beta, c)\) in Fig. 1.

Our simulation is carried out using population annealing Monte Carlo [36–40]. We initialize \( R \) random configurations or replicas of the same instance with a random boundary condition chosen from the 8 possible boundary conditions at \( \beta = 0 \). Define \( \mathcal{H} = \beta H \) as the reduced Hamiltonian. When we change the simulation parameters as in Fig. 1, or the reduced Hamiltonian from \( \mathcal{H} \) to \( \mathcal{H}' \), a replica is copied with the expectation number \( n_i = \exp[-(\mathcal{H}'_i - \mathcal{H}_i)/Q]\), where the normalization \( Q = (1/R) \sum_{i=1} \exp[-(\mathcal{H}'_i - \mathcal{H}_i)]\), to maintain the population size approximately the same as \( R \). In our simulation, the number of copies is either the floor or the ceiling of \( n_i \) with proper probabilities, to minimize fluctuations. After this resampling step, \( N_S \) sweeps using the Metropolis algorithm is applied to each replica. The
FIG. 1: Schematic simulation paths for temperature chaos and bond chaos. In all cases, an annealing from $\beta = 0$ to $T = T_C/2$ is performed. For temperature chaos, the path goes straight down in temperature reaching $T = T_C$. For bond chaos, the path turns horizontally into the $c$ direction at a constant $T = T_C/2$. When equilibration criteria are not met for an instance, we rerun it with a larger population size or more sweeps. However, if an instance is too chaotic to equilibrate in the $c$-path, then spending more computational work becomes impractical. The path is then split into two (or more, two are shown here) paths, which are later combined or number of temperature steps (evenly spaced in $\beta$) and $N_c$ is the number of disorder steps (evenly spaced in $c$) in the annealing schedule, and $M$ is the number of instances studied. We apply $N_S = 10$ sweeps to each replica after each annealing step.

| $BC$  | $TB$  | $L$       | $R$       | $T_{\text{min}}$ | $N_T$ | $N_c$ | $M$   |
|-------|-------|-----------|-----------|-------------------|-------|-------|-------|
| PTBC  | TC    | $2 \times 10^3$ | 0.6       | 101               | -     |       | 2000  |
| PTBC  | TC    | $6 \times 10^3$ | 0.6       | 201               | -     |       | 2000  |
| PTBC  | TC    | $2 \times 10^6$ | 0.6       | 301               | -     |       | 2000  |
| PTBC  | BC    | $2 \times 10^3$ | 0.9       | 101               | 51    |       | 2000  |
| PTBC  | BC    | $6 \times 10^3$ | 0.9       | 201               | 51    |       | 2000  |
| PTBC  | BC    | $2 \times 10^6$ | 0.9       | 301               | 101   |       | 2000  |

In this section, we summarize the scaling relations used in this work in the framework of the droplet picture. Flip boundary conditions create a relative domain wall between two boundary conditions. There are two scaling exponents in the droplet picture for such domain walls: the domain-wall free energy exponent $\theta$ and the domain-wall fractal dimension $d_s \in [d-1, d]$. Let $\Delta F$ be the free energy cost of inserting a domain wall and $\Sigma$ is the size or number of spins of the domain wall, then

$$\Delta F \sim L^\theta,$$

$$\Sigma \sim L^{d_s}. \quad (4)$$

Naturally $\Delta F = 0$ at a boundary condition crossing, but both $\Delta E$ and $T\Delta S$ are nontrivial like in a first-order phase transition and they scale as:

$$\Delta E \sim L^{d_s/2}, \quad (5)$$

$$T\Delta S \sim L^{d_s/2}. \quad (6)$$

Here it is simply assumed the scales are related to the size of domain walls (Eq. 5) and the square roots come from the frustrations of domain walls. Doing a Taylor expansion in the vicinity of a crossing for the generalized parameter $Q$ at $Q_0$ (either $Q = T$ for temperature chaos and bond chaos. In all cases, an annealing from $\beta = 0$ to $T = T_C/2$ is performed. For temperature chaos, the path goes straight down in temperature reaching $T = T_C$. For bond chaos, the path turns horizontally into the $c$ direction at a constant $T = T_C/2$. When equilibration criteria are not met for an instance, we rerun it with a larger population size or more sweeps. However, if an instance is too chaotic to equilibrate in the $c$-path, then spending more computational work becomes impractical. The path is then split into two (or more, two are shown here) paths, which are later combined or number of temperature steps (evenly spaced in $\beta$) and $N_c$ is the number of disorder steps (evenly spaced in $c$) in the annealing schedule, and $M$ is the number of instances studied. We apply $N_S = 10$ sweeps to each replica after each annealing step.

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or \( Q = c \) for bond chaos) gives:

\[
\Delta F(Q_0 + \delta Q) = \Delta F(Q_0) + \frac{\partial \Delta F}{\partial Q} \delta Q. \tag{8}
\]

\[
= \frac{\partial (\Delta E - T\Delta S)}{\partial Q} \delta Q. \tag{9}
\]

Suppose that \( \Delta E \) dominates the response to bond changes and \( T\Delta S \) dominates the response to temperature changes [17], we obtain:

\[
L^\theta \sim L^{d_s/2} \delta Q, \tag{10}
\]

\[
\delta Q \sim 1/L^\zeta, \tag{11}
\]

\[
\delta Q \sim 1/L^{d_s/2-\theta}, \tag{12}
\]

where \( \zeta = d_s/2 - \theta \) is the chaos exponent. Note that this is a derived exponent, depends on \( d_s \) and \( \theta \). In this work, we measure these three exponents independently for both forms of chaos and check this equality. One direct consequence of Eq. 11 is that the number of dominant boundary condition crossings \( N_C \) should scale as:

\[
N_C \sim L^\zeta, \tag{13}
\]

where a dominate boundary condition crossing is a crossing of two boundary conditions that also have the maximum weights. See the red circles in Fig. 2 for examples.

The exponent \( \theta \) can also be measured in the framework of thermal boundary conditions using the so-called sample stiffness scaling [15, 41]. In this approach, free energy is not measured directly like energy, although this is a derived exponent, depends on \( d_s \) and \( \theta \). In this work, we measure these three exponents independently for both forms of chaos and check this equality. One direct consequence of Eq. 11 is that the number of dominant boundary condition crossings \( N_C \) should scale as:

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The exponent \( \theta \) can also be measured in the framework of thermal boundary conditions using the so-called sample stiffness scaling [15, 41]. In this approach, free energy is not measured directly like energy, although this is also possible using the free energy perturbation method [36, 39]. Rather domain-wall free energy is conveniently estimated from the quantity sample stillness. For an instance at a temperature \( T \), it is defined as:

\[
\lambda(T) = \log \frac{p_{\text{max}}(T)}{1 - p_{\text{max}}(T)}, \tag{14}
\]

where \( p_{\text{max}} = \max\{p_i\} \) is the maximum weights of all the boundary conditions. Note that this is simply an estimator of the free-energy difference (times \( -\beta \)) between the dominant boundary condition and all other boundary conditions combined. Since \( p_{\text{max}} \) can be very close to 1 for some instances, and a precise estimation of \( \lambda \) for these instances would be difficult, one therefore usually works with a characteristic \( \lambda_{\text{char}} \) using a median, instead of the mean. The median is usually chosen from the tail of the distribution (large \( \lambda \)), but not too far into the tail where statistics are poor. In our work, we choose the 0.9 median and we have checked that our results are not sensitive to this particular choice. Naturally as Eq. 4, \( \lambda_{\text{char}} \) scales as:

\[
\lambda_{\text{char}} \sim L^\theta. \tag{15}
\]

We summarize our methods for measuring the scaling exponents: We use sample stiffness scaling (Eq. 15) to measure \( \theta \). At the boundary condition crossings \( \Delta F = 0 \), and we use \( \Delta E \) (Eq. 6) to measure \( d_s/2 \). We use only crossings that are above a threshold for good accuracy. For temperature chaos, we use crossings above \( p_c = 0.05 \). For bond chaos where there are more crossings, we use a slightly larger threshold \( p_c = 0.1 \). Our results, however, are not sensitive to these thresholds. We use the number of dominant crossings \( N_C \) (Eq. 13) to compute the exponent \( \zeta \). Note that the different thresholds do not affect \( N_C \), as no dominant crossings can occur below \( p = 0.125 \) with 8 boundary conditions. In the next Section, we present our results of temperature chaos and bond chaos, and the comparisons with the 3D model and the 4D \( \pm J \) model.

### III. RESULTS

#### A. Scaling properties of chaos

Chaos in (partial) thermal boundary conditions manifests as crossings of boundary condition weights, as shown in Fig. 2 for two typical moderately chaotic instances of size \( L = 6 \). The red circles and blue squares are examples of dominant crossings and crossings but not dominant ones, respectively. The histograms of those crossings above \( p_c \) for all instances of \( L = 6 \) are shown in Fig. 3. The distribution is approximately exponential with respect to \( \beta \) for temperature chaos, while uniform with respect to \( c \) for bond chaos. Our results clearly show that the effectiveness of temperature chaos decreases rapidly with decreasing temperature in the spin-glass phase. The uniform distribution of bond chaos is easy to understand because of the statistical symmetry of \( c \). The distributions are also very similar to their 3D counterparts, and see the next section for more quantitative comparisons.

One of our main results, the scalings of the sample stillness \( \lambda_{\text{char}}, \langle \Delta E \rangle \) at crossings, and the total number of dominant crossings \( N_C \) are shown in Fig. 4. Here, we have combined data at \( \beta = 2/T_c, c = 0 \) and \( \beta = 2/T_c, c = 0.1 \) to compute \( \theta \) to improve statistics, as the data at different \( c \) are statistically equivalent. Our estimates of the exponents are:

\[
\theta = 0.69(6) \tag{16}
\]

\[
d_s/2 = 1.74(3) \quad \text{(TC)} \tag{17}
\]

\[
d_s/2 - \theta = 1.05(7) \quad \text{(TC)} \tag{18}
\]

\[
\zeta = 1.19(7) \quad \text{(TC)} \tag{19}
\]

\[
d_s/2 = 1.84(4) \quad \text{(BC)} \tag{20}
\]

\[
d_s/2 - \theta = 1.15(7) \quad \text{(BC)} \tag{21}
\]

\[
\zeta = 1.20(6) \quad \text{(BC)}. \tag{22}
\]

The agreement of the exponents for TC and BC are reasonably good, and both are compatible with the relation \( \zeta = d_s/2 - \theta \). Therefore, we conclude temperature chaos and bond chaos share the same set of scaling exponents in four dimensions, as in three dimensions [17]. The
results also at the same time validate the partial thermal boundary condition technique for studying chaos.

Our estimate \( d_s/2 \) for TC is, however, somewhat smaller than that of BC, while the agreement of \( \zeta \) is excellent. One possible reason for this result is that there might be larger systematic errors for temperature chaos when averaging \( \langle |\Delta E| \rangle \) over a wide temperature range. In bond chaos, all quantities are averaged at a single temperature. By narrowing down the temperature range at low temperatures to only \( T = 0.8 \) or \( \beta = 1.25 \), the TC data set gives \( d_s/2 = 1.77(4) \), in good agreement with the BC result. Therefore, we believe our BC estimation of \( d_s \) and checking of the chaos equality are stronger. It is indeed the case that the relation \( \zeta = d_s/2 - \theta \) is in better agreement for bond chaos.

We now compare our results with the literature. Our stiffness exponent \( \theta = 0.69(6) \) is in good agreement with 0.61(2) using percolation method [42] and 0.64(5) using approximate ground states [43], both working at \( T = 0 \) for the \( \pm J \) model. Our estimate \( d_s \) is also in agreement with a recent result \( d_s \approx 3.74 \) using a strong disorder renormalization group method [44]. The chaos results are similar to that of Ref. [10], where chaos are studied for the \( \pm J \) model using correlation functions: \( \theta = 0.69(3) \), \( d_s/2 = 1.71(3) \), \( \zeta = 1.12(5) \) for temperature chaos and 1.10(10) for bond chaos. Our chaos exponents are slightly larger, but within errorbars.

One earlier work with Gaussian disorder is Ref. [31]. The author, however, separated two cases: Chaos at \( T_C \) and Chaos below \( T_C \). The results are \( \zeta = 0.85(10) \) for temperature chaos and \( \zeta = 0.95(20) \) for bond chaos at \( T_C \). Notice that they are compatible, even though they may differ from the exponent in the spin-glass phase. Below \( T_C \) in the spin-glass phase, only bond chaos was studied and \( \zeta = 1.2(1) \) at \( T = 1.4 \), also for sizes up to \( L = 7 \). This exponent is remarkably in good agreement with our results, even though the temperature is higher. All of these exponents are summarized for convenience in Table II. Take all these results collectively, we conclude also that the \( \pm J \) model has the same scaling exponents with Gaussian disorders in four dimensions.

### B. Relative strengths of chaos

Next, we compare the relative strength of temperature chaos and bond chaos at \( T_C/2 \), and also compare with that of 3D. We define density of crossings for both chaos, and the relative strength can be quantified as ratio of the densities. We follow the procedures established in Ref. [17] for three dimensions. The density of crossings for bond chaos is given by

\[
\rho^{BC} = \frac{N_C}{\beta \Delta c}
\]  
(23)

The distribution for temperature chaos is more complicated and is approximately exponential in the range...
TABLE II: Summary of exponents (relevant to chaos) of the four-dimensional EA model. Note that not all of these works are for studying chaos, but a few typical related results are presented for comparisons of $\theta$, $d_s$, and $\zeta$. Here, MC and GS stand for “Monte Carlo” and “Ground state”, respectively. We conclude that temperature chaos and bond chaos share the same set of chaos exponents, and the 4D EA spin glasses of Gaussian and $\pm J$ disorder also share the same set of chaos exponents.

| Reference | model   | result                                      | note                |
|-----------|---------|---------------------------------------------|---------------------|
| Ref. [31] | Gaussian | $\zeta = 0.85(10)$ (TC), $\zeta = 0.95(20)$ (BC) | MC, $T = T_C = 1.8$ |
| Ref. [31] | Gaussian | $\zeta = 1.2(1)$ (BC)                       | MC, $T = 1.4$       |
| This work | Gaussian | $\zeta = 1.19(7)$ (TC), $\zeta = 1.20(6)$ (BC) | MC, $T \approx T_C/2 = 0.9$ |
| This work | Gaussian | $\theta = 0.69(6)$, $d_s/2 = 1.74(3)$ (TC), $d_s/2 = 1.84(4)$ (BC) | MC, $T \approx T_C/2 = 0.9$ |
| Ref. [10] | $\pm J$  | $\zeta = 1.12(5)$ (TC), $\zeta = 1.10(10)$ (BC) | MC, $T \approx 0.6$ |
| Ref. [10] | $\pm J$  | $\theta = 0.69(3)$, $d_s/2 = 1.71(3)$ (TC)  | MC, $T \approx 0.6$ |
| Ref. [42] | $\pm J$  | $\theta = 0.61(2)$                         | percolation         |
| Ref. [43] | $\pm J$  | $\theta = 0.64(5)$                         | approximate GS     |
| Ref. [44] | Gaussian | $d_s = 3.7358(36)$                         | approximate GS     |

This work Gaussian

\[ \lambda_{cha} \sim L^\beta, \quad \langle |\Delta E| \rangle \sim L^{d_s/2} (TC), \quad N_C \sim L^\zeta (TC), \quad \langle |\Delta E| \rangle \sim L^{d_s/2} (BC), \quad N_C \sim L^\zeta (BC). \]

\[ \rho_{TC} = \frac{1.17 N_C^T}{\Delta \beta}. \]

Remarkably, the prefactor 1.17 depends only very weakly on $a$ and is very similar to that of the 3D 1.18 where bond chaos is again also studied at $\beta = 2/T_C$ [15, 17]. This therefore, provides also an excellent setting to compare the relative strength with the three dimensions, as we will do in the following.

The relative strength of bond chaos to temperature chaos is naturally defined as:

\[ \kappa = \frac{\rho_{BC}^T}{\rho_{TC}^T}, \]

\[ \approx 6.41 \frac{N_C^{BC}}{N_C^{TC}}, \]

where $N_C^{BC}$ and $N_C^{TC}$ are the total number of dominant boundary condition crossings of bond chaos and temperature chaos, respectively. The prefactor is again similar to three dimensions, where it is 6.34 [17]. A plot of $\kappa$ as a function of the linear system size $L$ is shown in Fig. 5.

Firstly, $\kappa$ is almost a constant function of $L$, as expected from the scaling properties of $N_C$. The interesting finding is that the relative strength is not a universal constant at the same scaled temperature $T = T_C/2$. Averaging over all studied system sizes, we get $\kappa = 9.5(1)$, compared with that of three dimensions 16(1). Ref. [10] got a value 17.5 for the 4D $\pm J$ model. While this appears to be rather close to that of the three dimensions instead as observed in Ref. [17], this is likely an interesting coincidence rather than suggesting the ratio is a universal constant at a typical low temperature. This large value is not in disagreement with our data as the value is calculated at a relatively lower temperature $0.3 T_C$. It is expected that $\kappa$ should increase with $\beta$. For example, bond chaos should persist even at $T = 0$, while for temperature chaos, this is likely negligibly small for the finite
sizes we have studied. Nevertheless, all of these data are fairly close, suggesting that bond chaos at a typical low temperature is almost an order of magnitude stronger than temperature chaos.

C. Does chaos imply many pure states?

It has long been believed the droplet picture [4, 26–29] is a two-state picture, as the exponent $\theta > 0$. However, numerical simulations have been observing nontrivial overlap distributions, i.e., many pure states. This is either interpreted as evidence for the replica symmetry breaking picture [45–47] or finite-size effect. It is beyond the scope of this paper to discuss fully this controversial topic, but now we focus on this question in the framework of thermal boundary conditions. In particular, we propose here a tentative view that the two-state picture may not hold from the perspective of chaos in the TBC ensemble argued as follows.

In fact, the primary motivation of the TBC [41] is exactly to study whether the overlap distribution function is trivial or not in the thermodynamic limit. Ref. [41] concluded the overlap distribution should become trivial using sample stiffness scalings. The basic idea is stiff instances (large $\lambda$) have trivial overlap distributions and all instances would become stiff in the thermodynamic limit. The paper, however, also stated though this may not occur if a fraction of instances are stiff $\Delta F \sim L^\theta$, while the others are not with $\Delta F \sim O(1)$ independent of $L$.

There had been no straightforward explanation for this scenario, but chaos appears to provide such a picture.

Our consideration comes from a confusing paradox: Suppose in the thermodynamic limit, one boundary condition dominates the ensemble as required by the droplet picture, but not the same one as temperature varies. If the boundary conditions are constantly exchanging their dominance, why would we always see one boundary condition whenever we make a measurement of their weights? We therefore propose the following picture for the thermodynamic limit as shown in Fig. 6. Clearly if $N_C \sim L^\xi$, each crossing event should scale as $1/L^\xi$. Each crossing event has two regimes: an $O(\ell^\theta)$ regime and an $O(1)$ regime in terms of free energy differences. In the former regime, one boundary condition dominates and the overlap distribution is trivial. In the latter regime, two (or more perhaps with a smaller probability) boundary conditions have comparable weights and the overlap distribution is nontrivial. The width of both regimes scales as $1/L^\xi$. Notice that excitations within a single boundary condition are not considered, which would only make the overlap distributions even less trivial.

At an arbitrarily fixed temperature, an instance may be randomly observed in either regime. When taking disorder averages, the exponent $\theta$ but a nontrivial overlap distribution function after taking disorder averages at any arbitrarily chosen temperature.
changes significantly at the tail of the distribution where $\Delta F$ is large. In our picture, this is naturally interpreted as the nonstiff instances are in the $O(1)$ regimes while the stiff instances are in the $O(\ell^0)$ regimes. Finally, Ref. [41] did find a nontrivial overlap distribution function.

We have recently heard, however, a possible way to save the droplet picture [48]. If for each crossing event, the $O(\ell^0)$ regime takes most of the share and the $O(1)$ regime has only a tiny share of $1/\ell^0$, then the total length of the $O(1)$ regimes would shrink as $1/\ell^0$. While this exotic scenario would again yield a two-state picture, we do not readily see an obvious reason for such uneven shares, and more importantly we do not seem to see such uneven shares or such a trend for the sizes we have studied. See Fig. 2 again for typical crossings which appear to look similar for all sizes. Moreover, the inversion from Eq. 11 to Eq. 13 would be less straightforward in this scenario. Nevertheless, we cannot exclude this scenario as a crossover in the thermodynamic limit.

IV. CONCLUSIONS & FUTURE CHALLENGES

In this work, we have successfully extended the thermal boundary condition technique to partial thermal boundary conditions, and applied it to study the temperature chaos and bond chaos of the four-dimensional Edwards-Anderson model with Gaussian disorder to low temperatures. We have measured the three scaling exponents of chaos, and found with good accuracy that they are related through the chaos equality of the droplet picture and the two forms of chaos share the same set of scaling exponents. Our results and the literature values also suggest that the scaling exponents are the same for the Gaussian disorder and the $\pm J$ model in four dimensions, unlike the two dimensions. Quantitative comparison of the relative strength of bond chaos and temperature chaos are also made at $T = T_C/2$ and compared with 3D, different but similar relative strengths are found. Temperature chaos distributions in 3D and 4D are also qualitatively similar, but nonetheless quantitatively different with the 4D has a larger exponent in the exponential distribution. We have also proposed a scenario that chaos may imply many pure states in the TBC ensemble.

Our results pave the way for the (partial) thermal boundary condition technique to be applied to a wide range of models, as the number of fluctuating boundary conditions can be chosen flexibly (up to factors of 2). For example, it is possible to use the method efficiently to study chaos of one-dimensional long-range models on a ring such as the mean-field Sherrington-Kirkpatrick model [49] by also keeping 8 boundary conditions by introducing three equally-spaced points as boundaries. In particular, the model also has a spin-glass phase in a magnetic field, and therefore temperature chaos, bond chaos and field chaos can be characterized and compared on the same footing. It is also straightforward and interesting to apply the method to other spin-lattice models such as Potts, clock, XY and Heisenberg spin glasses. Chaos of these models are far less studied but may exhibit new interesting phenomena. For example, the clock spin glasses can have an extremely rich phase diagram such as a chiral spin-glass phase, which is also chaotic [50]. Finally, we look forward to seeing Monte Carlo simulations of the Edwards-Anderson model in yet higher dimensions as a result of Moore’s law and parallel computing. Using the strong-disorder renormalization group $d_s$ [44] and the domain-wall stiffness exponent $\theta$ [42], we estimate $\zeta = 1.56(5)$ and $1.89(10)$ in five and six dimensions, respectively.

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