

This is the accepted manuscript made available via CHORUS. The article has been published as:

Numerical simulations of Ising spin glasses with free boundary conditions: The role of droplet excitations and domain walls

Wenlong Wang

Phys. Rev. E **95**, 032143 — Published 28 March 2017

DOI: [10.1103/PhysRevE.95.032143](https://doi.org/10.1103/PhysRevE.95.032143)

Numerical simulation of Ising spin glasses with free boundary conditions: the role of droplet excitations and domain walls

Wenlong Wang^{1,*}

¹*Department of Physics and Astronomy, Texas A&M University, College Station, Texas 77843-4242, USA*

The relative importance of the contributions of droplet excitations and domain walls on the ordering of short-range Edwards-Anderson spin glasses in three and four dimensions is studied. We compare the spin overlap distribution functions of periodic and free boundary conditions using population annealing Monte Carlo. For system sizes up to about 1000 spins, spin glasses show non-trivial spin overlap distributions. Periodic boundary conditions may trap diffusive domain walls which can contribute to small spin overlaps, and the other contribution is the existence of low-energy droplet excitations within the system. We use free boundary conditions to minimize domain-wall effects, and show that low-energy droplet excitations are the major contribution to small overlaps in numerical simulations. Free boundary conditions has stronger finite-size effects, and is likely to have the same thermodynamic limit with periodic boundary conditions.

I. INTRODUCTION

The nature of the ordering of short-range Edwards-Anderson (EA) spin glasses [1] is a subject of long-standing controversy [2–26]. The infinite-range Sherrington-Kirkpatrick (SK) model [27] is known to have an infinite number of pure states, described by replica symmetry breaking [28–30]. In the context of short-range spin glasses, there are two similar and plausible ways to have many pairs of pure states, but in terms of metastates [31–33]. For a finite large volume of spins, there might be one pair of pure states present, the chaotic pairs picture [33, 34] or many pairs of pure states, the non-standard replica symmetry breaking (RSB) picture [33, 35], both with chaotic size dependence and space-filling domain walls. The droplet picture on the other hand, developed by McMillan [36], Bray and Moore [37], as well as Fisher and Huse [38–40], is an example of the simple scenario that there is only a single pair of pure states and the thermodynamic limit is defined in the usual way. In the droplet/scaling picture, domain walls are fractal surfaces, not space-filling.

Many numerical simulations have been conducted to study the ordering of the EA model [2–5, 7–23, 26] with a confusing mixture of results, in particular whether domain walls are space-filling, and there is a finite weight near zero overlap in the spin overlap distribution function $P(q)$. According to the droplet/scaling picture, the free energy cost to flip a droplet of size ℓ scales as ℓ^θ , where $\theta > 0$ is the stiffness exponent, which is expected to be the same for domain-wall and droplet excitations. On the other hand, RSB predicts that $\theta = 0$ for droplet excitations. Consequently $P(0)$ scales as $\ell^{-\theta}$. Therefore, a finite $P(0)$ means there exist large-scale excitations in the system with $O(1)$ cost in free energy. Otherwise, there is a unique ordering of spins without system-size excitations. When a domain wall is created, there are ℓ^{d_s} spins on the surface of the domain wall, where d_s is the fractal dimension of the domain wall. In the droplet/scaling picture, the surface is a fractal with $D - 1 \leq d_s \leq D$, while in RSB the surface is space-filling and $d_s = D$, in D dimensions. To leading order

without finite-size corrections, domain walls appear to be fractals and the weights near zero overlap is finite [7, 8, 11, 14] for the system sizes currently accessible. New statistics or finite-size corrections are therefore intensively developed, and pointing to different scenarios [20, 23, 41–43].

In this work, we focus on the weights near zero overlap $P(0)$. *We are interested in the question: if the droplet/scaling picture holds, could it be that $P(0)$ is a finite constant trivially because of trapped diffusive domain walls in the usually applied periodic boundary conditions (PBC), or low-energy droplet excitations are the dominate contribution?* Note that boundary conditions is only relevant to the EA model, not the SK model. The motivation of the idea of diffusive domain walls is from the consideration that the overlap distribution function of the ferromagnetic Ising model is flat if antiperiodic boundary condition in the x -axis is applied, where the system traps topologically protected domain walls. For disordered systems like spin glasses, one can generalize this term by comparing the interfaces [44] of the thermodynamic states of the system, where an interface is a bond that is satisfied in one state but unsatisfied in the other state, i.e., a negative link overlap. If the interfaces are two percolating domain-wall surfaces (out of many depends on which two states are paired) at different locations of the system, then we say the system has trapped diffusive domain walls, which may be inserted at different locations, but with similar free energy cost. It is not hard to see that PBC may trap a diffusive domain wall that is topologically protected. On the other hand, such effects should be reduced for free boundary conditions (FBC). In this work, we use $P(0)$ as our primary observable, which is also sufficient, to detect the domain-wall effects instead of studying the complex interfaces at finite temperatures. We propose to compare $P(0)$ of PBC and FBC to answer the question. *Our strategy is as follows: (1) If domain-wall effects dominate, FBC should have stronger ordering than PBC as domain-wall effects are reduced, and (2) If droplet excitations dominate, FBC should make the ordering weaker or no change for finite systems, as droplet excitations are easier at the surface of the system.* In this context, a stronger ordering means a smaller $P(0)$ and a weaker ordering means a larger $P(0)$. To be more quantitative, if domain-wall effects dominate, we expect $P(0)$ to drop by a constant amount with little

*Electronic address: wenlongcmp@gmail.com

or no system size dependence as domain walls impact all system sizes in the same manner [26]. On the other hand, if droplet excitations dominate, the difference of $P(0)$ of PBC and FBC is expected to be a decreasing function of system size and converges to zero since the fraction of surface spins decreases to zero in the thermodynamic limit.

Thermal boundary conditions (TBC) [23] was used to reduce domain-wall effects, answered this question to some extent and indicated the answer is perhaps negative. The answer however is not completely clear, because TBC limits fluctuations only between periodic and antiperiodic boundary conditions according to the Boltzmann weights in each spatial direction, can still trap domain walls, and also overlaps between different boundary conditions are introduced. In this work, we minimize the domain-wall effects using FBC. FBC is probably the best boundary condition one can work with to separate the two effects. Our results show droplet excitations dominate $P(0)$, in line with that of TBC.

It is also well known that FBC introduces new finite-size effects as a substantial fraction of the spins are on the surface, which could be misleading when looking for a trend with limited system sizes. Therefore, it is crucial to compare FBC with PBC in interpreting the FBC data properly. FBC was used in the early work of Ref. [14] in revealing the nature of ordering of short-range spin glasses, and results for small system sizes were reported. In this work, we conduct large-scale Monte Carlo simulations, focusing in particular on $P(0)$ as a function of the system size in both three and four dimensions. The comparison of the PBC and FBC overlap functions suggests that they are likely to have the same thermodynamic limit. The existence of low-energy droplet excitations, and whether droplet excitations and domain walls have the same stiffness exponent have also been intensively studied. In Refs. [7, 45], a small perturbation is added to the Hamiltonian such that the ground state energy increases more than the excited states to detect changes in the ground state, and hence the existence of low-energy droplet excitations. In Ref. [46], various forms of droplet excitations are generated and the stiffness exponents are measured in two dimensions.

The paper is organized as follows. We first discuss the model, simulation methods and observables in Sec. II, followed by numerical results in Sec. III. Concluding remarks are stated in Sec. IV.

II. MODELS, METHODS AND OBSERVABLES

We study the three-dimensional (3D) and four-dimensional (4D) Edwards-Anderson Ising spin-glass model [1] defined by the Hamiltonian

$$H = - \sum_{\langle ij \rangle} J_{ij} S_i S_j, \quad (1)$$

where $S_i = \pm 1$ are Ising spins and the sum is over nearest neighbors on a hypercubic lattice of linear size L with number of spins $N = L^D$. The random couplings J_{ij} are chosen from a Gaussian distribution with mean 0 and variance 1. A set of couplings $\{J_{ij}\}$ defines a disorder realization. We apply

TABLE I: Simulation parameters for the 3D and 4D EA model using population annealing Monte Carlo. D is the dimension of the system, BC is the boundary condition, L is the linear system size, R_0 is the population size, T_0 is the lowest temperature simulated, N_T is the number of temperatures used in the annealing schedule, which is linear in β , and M is the number of disorder realizations studied. $N_S = 10$ sweeps are applied to each replica at each temperature.

D	BC	L	R_0	T_0	N_T	M
3	FBC	4	$5 \cdot 10^4$	0.20	101	5000
3	FBC	6	$2 \cdot 10^5$	0.20	101	5000
3	FBC	8	$5 \cdot 10^5$	0.20	201	5000
3	FBC	10	10^6	0.20	301	5000
3	FBC	12	10^6	0.33	301	5000
4	FBC	3	$2 \cdot 10^4$	0.36	101	5000
4	FBC	4	$5 \cdot 10^4$	0.36	101	5000
4	FBC	5	10^5	0.36	101	5000
4	FBC	6	$2 \cdot 10^5$	0.36	201	5000
4	FBC	7	$5 \cdot 10^5$	0.36	201	4400
4	FBC	8	$8 \cdot 10^5$	0.72	301	2000
4	PBC	3	$2 \cdot 10^4$	0.36	101	3000
4	PBC	4	$5 \cdot 10^4$	0.36	101	3000
4	PBC	5	10^5	0.36	101	3000
4	PBC	6	$2 \cdot 10^5$	0.36	201	3000
4	PBC	7	$5 \cdot 10^5$	0.36	201	3000
4	PBC	8	$8 \cdot 10^5$	0.72	301	3000

free boundary conditions, as well as periodic boundary conditions to each instance. The simulation is carried out using population annealing Monte Carlo [47–50]. The simulation parameters are summarized in Table I. Note that the transition temperatures are $T_C \approx 1$ in 3D [51] and $T_C \approx 1.8$ in 4D [52].

We study the spin overlap q defined as

$$q = \frac{1}{N} \sum_i S_i^{(1)} S_i^{(2)}, \quad (2)$$

where spin configurations “(1)” and “(2)” are chosen independently from the Boltzmann distribution, and its statistic $I(q_0)$

$$I(q_0) = \int_{-q_0}^{q_0} P(q) dq. \quad (3)$$

We study $I(0.2)$ unless otherwise specified.

III. RESULTS

In this section, we present our numerical results. We discuss the 3D results in Sec. III A and the 4D results in Sec. III B.

A. Three dimensions

The disorder-averaged spin overlap distributions $P(q)$ for periodic and free boundary conditions are shown in Fig. 1.

The data for PBC is taken from a previous study of Ref. [23]. Both display peaks at finite-size values of $\pm q_{\text{EA}}$, with the Edwards-Anderson order parameter q_{EA} decreases with L . For PBC at small q the distribution is nearly independent of L , consistent with many past studies [7, 11, 14, 20].

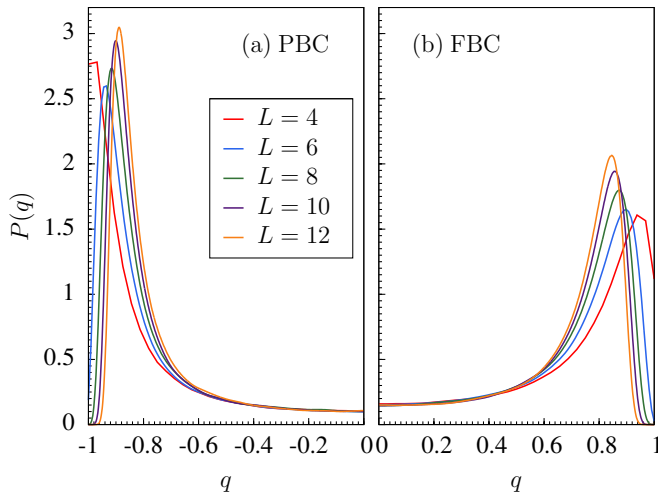


FIG. 1: (Color online) Disorder-averaged spin overlap distributions $P(q)$ in 3D for sizes $L = 4, 6, 8, 10$, and 12 at $T = 0.42$ with (a) periodic and (b) free boundary conditions. The finite-size values of $\pm q_{\text{EA}}$ decreases with system size. Note that FBC is less ordered than PBC for the system sizes studied.

The statistic I as a function of system sizes is shown in Fig. 2. We find that the FBC ordering gets *weaker* rather than stronger compared with PBC, with noticeable size corrections. This suggest that trapped domain walls in PBC cannot be used to argue why $P(0)$ is finite, and droplet excitations are at work. For very small system sizes, I appears to decrease with system size, similar to what was found in Ref. [14]. However, as system size gets larger, this trend does not appear to hold, especially at the lower temperature $T = 0.2$, PBC appears to provide a lower bound for FBC. The same appears to hold in 4D, as shown in the next section.

It is easy to understand why I is larger for small system sizes in FBC than PBC if droplet excitations dominate. If droplet/scaling picture holds, larger droplets can be excited by taking advantage of the free bonds on the surface. But I would eventually become trivially the same and become zero when system size gets larger, as the free energy cost inside the system would dominate and diverge, the free bonds on the surface will not help. If on the other hand RSB is correct, we again expect the excitations can take advantage of the free bonds on the surface, and expect this effect to be increasingly less important for larger system sizes. This would naturally suggest the same thermodynamic limit for FBC and PBC. Furthermore, the insensitivity of metastates to boundary conditions in the non-standard RSB [33, 35] with chaotic size dependence also supports the scenario that FBC and PBC have the same thermodynamic limit. Therefore, we believe that the PBC I is not only a lower bound for FBC, but the two would eventually become the same in the thermodynamic

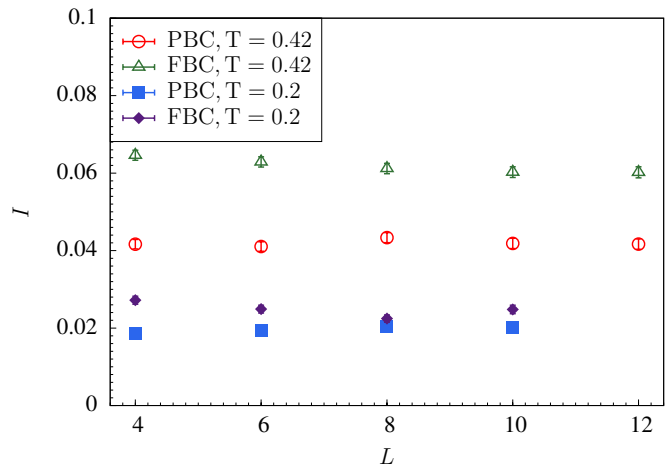


FIG. 2: (Color online) I as a function of system size L in 3D for periodic and free boundary conditions. I is approximately a constant for PBC, and is a fast decreasing function at small L for FBC, but appears to level off and is bounded by the values of the PBC when L increases.

limit. Our numerical results appear to support this conjecture, especially in 4D and lower temperatures, where finite-size effects are smaller.

B. Four dimensions

The overlap distribution $P(q)$ and the statistic I for PBC and FBC are shown in Figs. 3 and 4, respectively. Similar behaviours as in 3D are found except that the trend becomes more profound. By looking at I of FBC alone, one may would like to argue I is a decreasing function of L . However, we believe this is due the the strong finite-size effects of FBC. Note that in 3D, I is also a decreasing function of L up to around $L \approx 8$, and only appears to decrease slower or level off thereafter. We expect I of FBC is still bounded and will converge to that of PBC in 4D. It is easy to understand why the convergence is faster at lower temperatures, where thermal fluctuation is smaller. It is interesting that the convergence is faster in 4D than 3D when the temperatures are similar (both are around $0.4T_C$ and $0.2T_C$). This could be intuitively understood from the number of neighbours. For example for a spin on the interior of a surface, it will lose one neighbour out of a total of 8 neighbours in 4D but only 6 neighbours in 3D. Therefore, the effects of FBC will be a decreasing function of dimensionality, except for very small system sizes where the fraction of surface spins would dominate. This simple explanation is in agreement with the more quantitative/generic explanation that the correlation function decays faster in 4D or the sample stiffness exponent is much larger in 4D, as discussed in greater detail in the following text. This consideration gives more weight to our conjecture that the overlap distribution of FBC and PBC have the same thermodynamic limit, as finite-size effects are smaller in 4D than in 3D.

Finally we analyze quantitatively of our data with curve

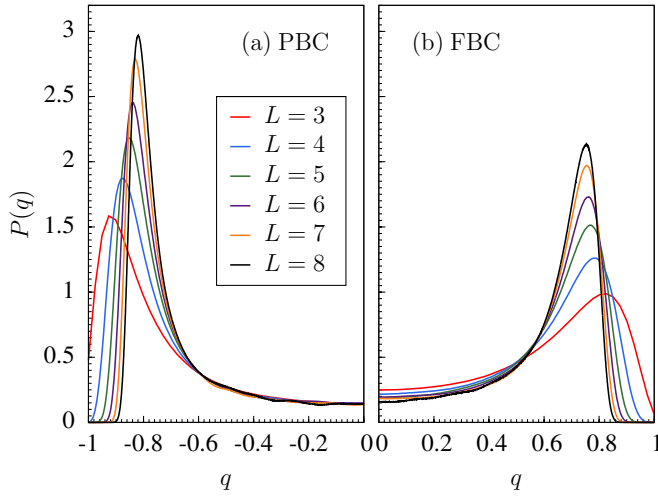


FIG. 3: (Color online) Disorder-averaged spin overlap distributions $P(q)$ in 4D for sizes $L = 3, 4, 5, 6, 7$, and 8 at $T = 0.72$ with (a) periodic and (b) free boundary conditions. The finite-size values of $\pm q_{\text{EA}}$ decreases with system size. Note that FBC is less ordered than PBC for the system sizes studied.

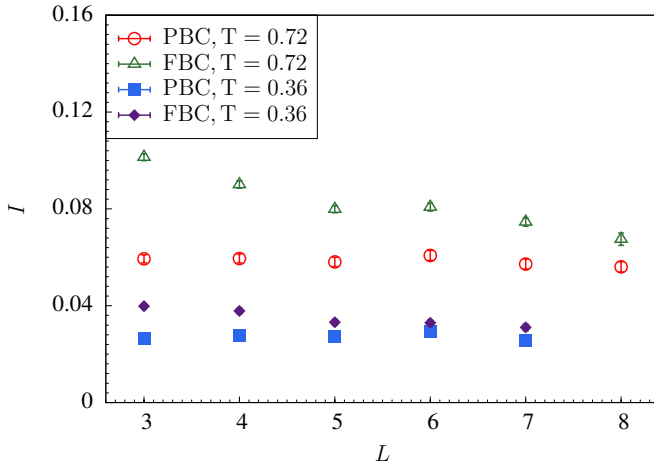


FIG. 4: (Color online) I as a function of system size L in 4D for periodic and free boundary conditions. I is approximately a constant for PBC, and is a fast decreasing function of L for FBC, but appears to level off and is bounded by the values of the PBC when L increases. The fluctuation at $L = 5$ and 6 is likely due to even-odd effects for small system sizes.

fitting using ansatz scalings of both the RSB and the droplet/scaling pictures. The goal is to test if the asymptotic values of I of PBC and FBC are the same, and also which picture our data fits best. We use the following scaling functions:

$$I_{\text{RSB}} = a_1/L^{\theta'} + c, \quad (4)$$

$$I_{\text{DS}} = a_2/L^b, \quad (5)$$

for RSB fits and droplet/scaling fits, respectively.

The exponent θ' within the RSB theory, controls the algebraic decay of the correlation function within the $q = 0$ sector.

We use the known exponents $\theta' = 0.38(2)$ in 3D [19, 53] and $\theta' = 1.0(1)$ in 4D [54] to reduce the degree of freedom. For the droplet/scaling picture, one may would like to use the stiffness exponent θ which is $\theta \approx 0.2$ in 3D [23] and $\theta \approx 0.7$ in 4D [55, 56]. However, these fits are going to be poor as one can easily see especially for PBC that such strong decays do not present for the system sizes accessible. Therefore, we relax this exponent as a fitting parameter b . In this way, one can compare b with θ to see if the $1/\ell^\theta$ decay is observed. Note that this also makes both fits having two fitting parameters. The results are listed in Table. II.

One interesting result is in the c column. We see the asymptotic I of PBC and FBC with the RSB fits are compatible within statistical errors, in agreement with our conjecture. On the other hand, I would become 0 for the droplet/scaling picture by construction. The goodness of fits Q for RSB and droplet/scaling are similar. However, some of the exponents b have very large statistical errors, suggesting the absences of the $1/\ell^\theta$ decay. Furthermore, the exponents b are far from θ . Therefore, it is reasonable to conclude the data fits the RSB picture better than the droplet/scaling picture.

IV. CONCLUSIONS AND FUTURE CHALLENGES

In this work, we studied whether the finite $P(0)$ observed in numerical simulations of the EA model in 3D and 4D is dominated by domain walls or droplet excitations. To this effort, we compared the spin overlap distribution functions of periodic and free boundary conditions, as the two effects make dramatically different predictions for $P(0)$ when we change the boundary conditions from PBC to FBC. Our results suggest that droplet excitations, not domain walls are the main contribution to small overlaps. Our data at different temperatures and dimensions also suggests that the overlap distributions of PBC and FBC are likely to have the same thermodynamic limit. A rigorous proof of this would be interesting, yet challenging as FBC is not gauge related to PBC.

If we believe in this conjecture, our results show that the initial decrease of $P(0)$ of FBC is a result of finite-size effects, not the onset of the droplet/scaling picture. Therefore, our data for the statistic I in FBC is still a support of the RSB picture, as in PBC. Furthermore, our results indicate that it is important to compare FBC with PBC for future studies with FBC to avoid misleading conclusions due to the strong finite-size effects of FBC.

Acknowledgments

W.W. would like to thank D. L. Stein, M. A. Moore, J. Machta and H. G. Katzgraber for fruitful discussions and comments on an earlier version of the manuscript. W.W. acknowledges support from NSF-DMR-1151387. The work is supported in part by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via MIT Lincoln Laboratory Air Force Contract No. FA8721-05-C-0002. The views and conclusions

TABLE II: Fitting parameters of the RSB and droplet/scaling fits of the statistic I using Eqs. 4 and 5. D is the dimensionality, T is the temperature, BC is the boundary condition, a_1, a_2, b, c are fitting parameters, and Q_1, Q_2 are the goodness of fits.

D	T	BC	a_1	c	Q_1	a_2	b	Q_2
3	0.42	FBC	0.0235(33)	0.0508(16)	0.9837	0.0709(16)	0.0684(111)	0.9759
3	0.42	PBC	-0.0023(98)	0.0430(46)	0.6468	0.0405(55)	-0.0267(660)	0.2688
3	0.20	FBC	0.0185(259)	0.0158(129)	0.0794	0.0323(123)	0.1364(2008)	0.0614
3	0.20	PBC	0.0098(71)	0.0244(35)	0.8520	0.0162(35)	-0.1092(1107)	0.6591
4	0.72	FBC	0.1540(240)	0.0509(49)	0.0311	0.1542(133)	0.3856(522)	0.0386
4	0.72	PBC	0.0123(141)	0.0560(29)	0.6381	0.0635(52)	0.0489(478)	0.6777
4	0.36	FBC	0.0475(115)	0.0246(26)	0.5065	0.0558(58)	0.2975(671)	0.5548
4	0.36	PBC	-0.0029(176)	0.0279(39)	0.3927	0.0261(69)	-0.0150(1632)	0.3087

contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the U.S. Government. The U.S. Government is authorized

to reproduce and distribute reprints for Governmental purpose notwithstanding any copyright annotation thereon. We thank Texas A&M University for access to their Ada and Curie clusters.

-
- [1] S. F. Edwards and P. W. Anderson, *Theory of spin glasses*, J. Phys. F: Met. Phys. **5**, 965 (1975).
- [2] M. Mézard, G. Parisi, N. Sourlas, G. Toulouse, and M. Virasoro, *Nature of the Spin-Glass Phase*, Phys. Rev. Lett. **52**, 1156 (1984).
- [3] M. A. Moore, H. Bokil, and B. Drossel, *Evidence for the droplet picture of spin glasses*, Phys. Rev. Lett. **81**, 4252 (1998).
- [4] B. Drossel, H. Bokil, M. A. Moore, and A. J. Bray, *The link overlap and finite size effects for the 3d Ising spin glass*, Euro. Phys. J. **13**, 369 (2000).
- [5] F. Krzakala and O. C. Martin, *Spin and link overlaps in 3-dimensional spin glasses*, Phys. Rev. Lett. **85**, 3013 (2000).
- [6] M. Palassini and A. P. Young, *Triviality of the ground state structure in Ising spin glasses*, Phys. Rev. Lett. **83**, 5126 (1999).
- [7] M. Palassini and A. P. Young, *Nature of the spin glass state*, Phys. Rev. Lett. **85**, 3017 (2000).
- [8] E. Marinari and G. Parisi, *On the effects of changing the boundary conditions on the ground state of Ising spin glasses*, Phys. Rev. B **62**, 11677 (2000).
- [9] E. Marinari, G. Parisi, F. Ricci-Tersenghi, J. J. Ruiz-Lorenzo, and F. Zuliani, *Replica symmetry breaking in short range spin glasses: A review of the theoretical foundations and of the numerical evidence*, J. Stat. Phys. **98**, 973 (2000).
- [10] E. Marinari, G. Parisi, F. Ricci-Tersenghi, and J. J. Ruiz-Lorenzo, *Off-equilibrium dynamics at very low temperatures in three-dimensional spin glasses*, J. Phys. A **33**, 2373 (2000).
- [11] H. G. Katzgraber, M. Palassini, and A. P. Young, *Monte Carlo simulations of spin glasses at low temperatures*, Phys. Rev. B **63**, 184422 (2001).
- [12] A. A. Middleton, *Energetics and geometry of excitations in random systems*, Phys. Rev. B **63**, 060202(R) (2001).
- [13] N. Hatano and J. E. Gubernatis, *Evidence for the droplet picture in the 3d $\pm J$ spin glass*, Phys. Rev. B **66**, 054437 (2002).
- [14] H. G. Katzgraber and A. P. Young, *Monte Carlo simulations of spin-glasses at low temperatures: Effects of free boundary conditions*, Phys. Rev. B **65**, 214402 (2002).
- [15] H. G. Katzgraber and A. P. Young, *Monte Carlo studies of the one-dimensional Ising spin glass with power-law interactions*, Phys. Rev. B **67**, 134410 (2003).
- [16] H. G. Katzgraber and A. P. Young, *Geometry of large-scale low-energy excitations in the one-dimensional Ising spin glass with power-law interactions*, Phys. Rev. B **68**, 224408 (2003).
- [17] G. Hed and E. Domany, *Nontrivial link overlap distribution in three-dimensional Ising spin glasses*, Phys. Rev. B **76**, 132408 (2007).
- [18] L. Leuzzi, G. Parisi, F. Ricci-Tersenghi, and J. J. Ruiz-Lorenzo, *Diluted One-Dimensional Spin Glasses with Power Law Decaying Interactions*, Phys. Rev. Lett. **101**, 107203 (2008).
- [19] R. Alvarez Baños, A. Cruz, L. A. Fernandez, J. M. Gil-Narvion, A. Gordillo-Guerrero, M. Guidetti, A. Maiorano, F. Mantovani, E. Marinari, V. Martin-Mayor, et al., *Nature of the spin-glass phase at experimental length scales*, J. Stat. Mech. P06026 (2010).
- [20] B. Yucesoy, H. G. Katzgraber, and J. Machta, *Evidence of Non-Mean-Field-Like Low-Temperature Behavior in the Edwards-Anderson Spin-Glass Model*, Phys. Rev. Lett. **109**, 177204 (2012).
- [21] A. Billoire, L. A. Fernandez, A. Maiorano, E. Marinari, V. Martin-Mayor, G. Parisi, F. Ricci-Tersenghi, J. J. Ruiz-Lorenzo, and D. Yllanes, *Comment on "Evidence of Non-Mean-Field-Like Low-Temperature Behavior in the Edwards-Anderson Spin-Glass Model"*, Phys. Rev. Lett. **110**, 219701 (2013).
- [22] B. Yucesoy, H. G. Katzgraber, and J. Machta, *Yucesoy, Katzgraber, and Machta reply*, Phys. Rev. Lett. **110**, 219702 (2013).
- [23] W. Wang, J. Machta, and H. G. Katzgraber, *Evidence against a mean-field description of short-range spin glasses revealed through thermal boundary conditions*, Phys. Rev. B **90**, 184412 (2014).
- [24] W. Wang, J. Machta, and H. G. Katzgraber, *Chaos in spin glasses revealed through thermal boundary conditions*, Phys. Rev. B **92**, 094410 (2015).
- [25] W. Wang, J. Machta, and H. G. Katzgraber, *Bond chaos in spin glasses revealed through thermal boundary conditions*, Phys. Rev. B **93**, 224414 (2016).
- [26] T. Aspelmeyer, W. Wang, M. A. Moore, and H. G. Katzgraber, *Interface free-energy exponent in the one-dimensional Ising spin glass with long-range interactions in both the droplet and*

- broken replica symmetry regions*, Phys. Rev. E **94**, 022116 (2016).
- [27] D. Sherrington and S. Kirkpatrick, *Solvable model of a spin glass*, Phys. Rev. Lett. **35**, 1792 (1975).
- [28] G. Parisi, *Infinite number of order parameters for spin-glasses*, Phys. Rev. Lett. **43**, 1754 (1979).
- [29] G. Parisi, *The order parameter for spin glasses: a function on the interval 0–1*, J. Phys. A **13**, 1101 (1980).
- [30] G. Parisi, *Order parameter for spin-glasses*, Phys. Rev. Lett. **50**, 1946 (1983).
- [31] M. Aizenman and J. Wehr, *Rounding effects of quenched randomness on first-order phase transitions*, Comm. Math. Phys. **130**, 489 (1990).
- [32] C. M. Newman and D. L. Stein, *Spatial Inhomogeneity and Thermodynamic Chaos*, Phys. Rev. Lett. **76**, 4821 (1996).
- [33] C. M. Newman and D. L. Stein, *Metastate approach to thermodynamic chaos*, Phys. Rev. E **55**, 5194 (1997).
- [34] C. M. Newman and D. L. Stein, *Multiple states and thermodynamic limits in short-ranged Ising spin-glass models*, Phys. Rev. B **46**, 973 (1992).
- [35] N. Read, *Short-range Ising spin glasses: the metastate interpretation of replica symmetry breaking*, Phys. Rev. E **90**, 032142 (2014).
- [36] W. L. McMillan, *Domain-wall renormalization-group study of the two-dimensional random Ising model*, Phys. Rev. B **29**, 4026 (1984).
- [37] A. J. Bray and M. A. Moore, *Scaling theory of the ordered phase of spin glasses*, in *Heidelberg Colloquium on Glassy Dynamics and Optimization*, edited by L. Van Hemmen and I. Morgenstern (Springer, New York, 1986), p. 121.
- [38] D. S. Fisher and D. A. Huse, *Ordered phase of short-range Ising spin-glasses*, Phys. Rev. Lett. **56**, 1601 (1986).
- [39] D. S. Fisher and D. A. Huse, *Absence of many states in realistic spin glasses*, J. Phys. A **20**, L1005 (1987).
- [40] D. S. Fisher and D. A. Huse, *Equilibrium behavior of the spin-glass ordered phase*, Phys. Rev. B **38**, 386 (1988).
- [41] A. A. Middleton, *Extracting thermodynamic behavior of spin glasses from the overlap function*, Phys. Rev. B **87**, 220201 (2013).
- [42] C. Monthus and T. Garel, *Typical versus averaged overlap distribution in spin glasses: Evidence for droplet scaling theory*, Phys. Rev. B **88**, 134204 (2013).
- [43] M. Wittmann, B. Yucesoy, H. G. Katzgraber, J. Machta, and A. P. Young, *Low-temperature behavior of the statistics of the overlap distribution in Ising spin-glass models*, Phys. Rev. B **90**, 134419 (2014).
- [44] D. L. Stein and C. M. Newman, *Spin Glasses and Complexity*, Primers in Complex Systems (Princeton University Press, 2013).
- [45] A. K. Hartmann and A. P. Young, *Large-scale low-energy excitations in the two-dimensional Ising spin glass*, Phys. Rev. B **66**, 094419 (2002).
- [46] A. K. Hartmann and M. A. Moore, *Generating droplets in two-dimensional Ising spin glasses using matching algorithms*, Phys. Rev. B **69**, 104409 (2004).
- [47] K. Hukushima and Y. Iba, in *The Monte Carlo method in the physical sciences: celebrating the 50th anniversary of the Metropolis algorithm*, edited by J. E. Gubernatis (AIP, 2003), vol. 690, p. 200.
- [48] E. Zhou and X. Chen, in *Proceedings of the 2010 Winter Simulation Conference (WSC)* (2010), p. 1211.
- [49] J. Machta, *Population annealing with weighted averages: A Monte Carlo method for rough free-energy landscapes*, Phys. Rev. E **82**, 026704 (2010).
- [50] W. Wang, J. Machta, and H. G. Katzgraber, *Population annealing: Theory and application in spin glasses*, Phys. Rev. E **92**, 063307 (2015).
- [51] H. G. Katzgraber, M. Körner, and A. P. Young, *Universality in three-dimensional Ising spin glasses: A Monte Carlo study*, Phys. Rev. B **73**, 224432 (2006).
- [52] G. Parisi, F. Ricci-Tersenghi, and J. J. Ruiz-Lorenzo, *Equilibrium and off-equilibrium simulations of the 4d Gaussian spin glass*, J. Phys. A **29**, 7943 (1996).
- [53] F. Belletti, A. Cruz, L. A. Fernandez, A. Gordillo-Guerrero, M. Guidetti, A. Maiorano, F. Mantovani, E. Marinari, V. Martin-Mayor, J. Monforte, et al., *An In-Depth View of the Microscopic Dynamics of Ising Spin Glasses at Fixed Temperature*, Journal of Statistical Physics **135**, 1121 (2009).
- [54] L. Nicolao, G. Parisi, and F. Ricci-Tersenghi, *Spatial correlation functions and dynamical exponents in very large samples of four-dimensional spin glasses*, Phys. Rev. E **89**, 032127 (2014).
- [55] S. Boettcher, *Stiffness exponents for lattice spin glasses in dimensions $d = 3, \dots, 6$* , The European Physical Journal B - Condensed Matter and Complex Systems **38**, 83 (2004).
- [56] K. Hukushima, *Domain-wall free energy of spin-glass models: Numerical method and boundary conditions*, Phys. Rev. E **60**, 3606 (1999).