

Numerical Construction of the Aizenman-Wehr Metastate

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Chaotic size dependence makes it extremely difficult to take the thermodynamic limit in disordered systems. Instead, the metastate, which is a distribution over thermodynamic states, might have a smooth limit. So far, studies of the metastate have been mostly mathematical. We present a numerical construction of the metastate for the $d = 3$ Ising spin glass. We work in equilibrium, below the critical temperature. Leveraging recent rigorous results, our numerical analysis gives evidence for a dispersed metastate, supported on many thermodynamic states.

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Introduction.—Symmetry breaking and phase transitions are well defined for systems of infinite size, $L = \infty$. Indeed, $L = \infty$ states can be defined rigorously as Dobrushin-Lanford-Ruelle (DLR) states [1]. However, experiments are conducted on systems of very large, but finite size. Therefore, one would like to interpret DLR states as the $L \rightarrow \infty$ limit of states defined on a sequence of systems of growing size. Indeed, for simple systems, e.g., ferromagnets, we know how to approach DLR states with finite- L states by using suitable boundary conditions. Yet, for disordered systems [2,3], the connection between DLR and finite- L states is still much of a mystery [4], most particularly for spin glasses [5–9].

For the sake of concreteness, let us consider the standard model for spin glasses, the Edwards-Anderson (EA) model [10] in spatial dimension d . Ising spins $s_i = \pm 1$, located in a size L cube, $\Lambda_L \subset \mathbb{Z}^d$ (see Fig. 1), interact through a nearest neighbor, bond disordered, and strongly frustrated Hamiltonian,

$$H_{\mathcal{J},L}(\underline{s}) = -\sum_{\langle i,j \rangle} J_{ij} s_i s_j. \quad (1)$$

The quenched couplings J_{ij} are independent and identically distributed random variables ($J_{ij} = \pm 1$ with 50% probability, in our case). We call $\mathcal{J} \equiv \{J_{ij}\}$ a disorder sample. The finite- L Gibbs state $\Gamma_{\mathcal{J},L}(\underline{s}) = \exp[-H_{\mathcal{J},L}(\underline{s})/T]/Z_{\mathcal{J},L}$ is a random state, as it depends on the set of random couplings \mathcal{J} .

The problem in taking the large L limit for spin glasses defined by Eq. (1) is caused by their chaotic size dependence. Take a fixed, arbitrary yet finite region (e.g., the measuring window Λ_W in Fig. 1). The Gibbs measure over

Λ_W changes chaotically when the system grows by the addition of new couplings at the boundaries, while keeping previous couplings unaltered. This extreme sensibility to changes at the boundaries motivated the invention of the metastate [5], a probability distribution over states with a (hopefully) smoother $L \rightarrow \infty$ limit.

The two main metastate definitions are those of Aizenman and Wehr (AW) [4] and Newman and Stein [5]. We focus on the former (the two definitions are conjectured to be equivalent [6], but that of AW is easier to implement numerically). The lattice Λ_L in Fig. 1 is divided into an inner region Λ_R , a cube of linear size R , and an outer region. Consequently we call internal couplings the set $\mathcal{I} \equiv \{J_{ij}|i, j \in \Lambda_R\}$ and outer couplings $\mathcal{O} = \mathcal{J} \setminus \mathcal{I}$. We proceed by (i) restricting our attention to the measuring window Λ_W of linear size W [9], (ii) taking the average over the outer couplings, with fixed internal couplings, and (iii) sending to infinity all three length scales while respecting $W \ll R \ll L$. If the limit of a translation invariant quantity exists (which is yet to be proven), it is independent of the arbitrary choice for the fixed internal couplings [11].

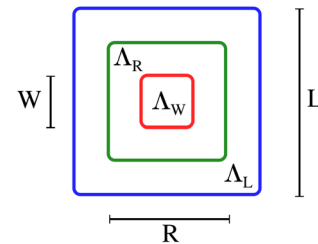


FIG. 1. Sketch of the AW metastate construction.

Yet, even if at a considerably lesser level of mathematical rigor, we must recall that there has been some progress in the study of spin glasses. We have numerical [12,13] and experimental [14] evidences for the existence of a phase transition to a spin-glass phase at low temperatures in $d = 3$, at least in the absence of an external magnetic field. We also have two major theoretical frameworks that are applied to interpret experiments and simulations: the replica symmetry breaking (RSB) theory [15,16] and the droplet model [17–19]. Which (if any) of these two theories captures the nature of the spin-glass phase in $d = 3$ is being debated [20].

In fact, a recent mathematical tour de force [21–23] has shown that the RSB theory provides the exact solution to the $d = \infty$ Sherrington-Kirkpatrick model [24]. The common lore expects RSB to be also valid above and at the upper critical dimension $d_U = 6$. RSB theory extends as well to $d < d_U$ features found in the mean field solution [25]: many states (infinitely many in the $L \rightarrow \infty$ limit), hierarchically organized, contribute to the Gibbs measure, each one with a weight that depends on the disorder realization. Consequences include the existence of the de Almeida-Thouless line [26] (the spin-glass phase transition survives in the presence of a small external magnetic field [27]), or the strong sample-to-sample fluctuations induced by the nonself-averageness of several measurable quantities [28] (these observations [27,28] were, however, obtained by simulating systems of finite size).

The alternative droplet model provides a much simpler scenario for the spin-glass phase, where the Gibbs measure is a mixture of two spin-flip related pure states. It follows that the spin-glass phase transition should disappear when a magnetic field is applied [the field breaks the global spin-flip symmetry $H(\underline{s}) = H(-\underline{s})$ in Eq. (1)].

The most recent mathematical analysis, based on metastates, has critically assessed both the RSB theory and the droplet model. Currently, we have three mathematically consistent pictures for the spin-glass phase. First, the droplet model metastate is concentrated on a single trivial state (let us call trivial a state that is a mixture of two pure states related by the global spin-flip symmetry). Second, we have the chaotic pairs picture [5,7], predicting a disperse metastate (there is a large number of states to choose from), yet each state is trivial. This nontrivial metastate is due to chaotic size dependence: by gradually increasing L , one obtains vastly different states. Finally, the RSB metastate [9] is disperse and every state drawn from it contains the Parisi hierarchical tree of pure states. Alternatives to these three pictures are much limited by recent rigorous results [29].

Read argues [9] that one can partially discriminate between these competing pictures for the metastate by studying the decay of a particular correlation function averaged over the metastate, $C_\rho(x) \sim 1/|x|^{d-\zeta}$ for large distances $|x|$; see Eq. (2). An exponent value $\zeta < d$ implies a disperse metastate, thus ruling out the droplet model's

metastate. Furthermore, in the context of the RSB metastate, the number of pure states that can be resolved by studying a region of size W is exponentially large in $W^{d-\zeta}$.

To the best of our knowledge there has been only one numerical attempt to study the metastate, by means of a nonequilibrium simulation [30]. Yet, the main debated points regard the equilibrium metastate. In fact, the only related issue addressed numerically by equilibrium simulations has been nonself-averageness [20,28,31–33].

Here we show that a numerical construction of the Aizenman and Wehr metastate for the Edwards-Anderson model in $d = 3$ is possible in present-day computers. Our construction makes precise several hints by Read [9]. In particular, recall Fig. 1, we show how big the ratios of length scales L/R , R/W need to be to uncover metastate properties. We also study the dependence on the fixed internal couplings, a crucial issue that has not yet been addressed quantitatively. We make quantitative computations of overlap distributions and correlation functions averaged over the AW metastate, thus computing the crucial ζ exponent. We find a value definitively smaller than $d = 3$, which rules out the droplet model metastate and leaves the chaotic pairs and the RSB metastates as the remaining contenders.

Metastate averages and the Metastate-averaged state.— In the context depicted by Fig. 1, we consider model (1) endowed with periodic boundary conditions (which makes irrelevant the location of Λ_R in Λ_L). Let us consider the probability distribution of $\Gamma_{\mathcal{J},L}$ at fixed internal disorder \mathcal{I} , while sending $L \rightarrow \infty$ and averaging over the outer disorder \mathcal{O} ,

$$\kappa_{\mathcal{I},R}(\Gamma) = \lim_{L \rightarrow \infty} \mathbb{E}_{\mathcal{O}}[\delta^{(F)}(\Gamma - \Gamma_{\mathcal{J},L})]$$

If the limit $\kappa(\Gamma) = \lim_{R \rightarrow \infty} \kappa_{\mathcal{I},R}(\Gamma)$ exists, it no longer depends on the internal disorder \mathcal{I} and provides the AW metastate. The purpose of the measuring window Λ_W in Fig. 1 is avoiding boundary effects that may appear as long as R is finite. Any measure is taken only inside Λ_W , while bonds are fixed in Λ_R in the metastate definition.

We have two kinds of averages, thermal averages over the Gibbs state $\langle \dots \rangle_\Gamma$ and averages over the metastate $[\dots]_\kappa$, that can be combined in different ways. For example, the metastate-averaged state (MAS) $\rho(\underline{s})$ is defined via the average $\langle \dots \rangle_\rho \equiv [\langle \dots \rangle_\Gamma]_\kappa$.

As seen from the measuring window Λ_W , a state $\Gamma(\underline{s})$ is a set of probabilities $\{p_\alpha\}_{\alpha=1,\dots,2^{Wd}}$ over the spin configurations in Λ_W . In other words, it is a point on the hyperplane defined by the equation $\sum_\alpha p_\alpha = 1$, $p_\alpha \geq 0$. In this sense, the metastate is a probability distribution over this hyperplane. The MAS $\rho(\underline{s})$ is the average of this distribution, and it is itself a point on the hyperplane (hence, the MAS is a state itself).

The numerical construction of the metastate.—We simulate the EA model ($8 \leq L \leq 24$) sampling spin

configurations at equilibrium by a combination of Metropolis single spin-flip Monte Carlo simulations and parallel tempering [34]. All the data shown are measured at the lowest simulated temperature $T = 0.698 \approx 0.64T_c$, well below the critical temperature $T_c = 1.102(3)$ [35]. Equilibration was assessed on a sample-by-sample basis [36] and, for the largest systems, it required the use of multisite multispin coding [37] (see [38] for details).

We repeat the computation for $\mathcal{N}_{\mathcal{I}} = 10$ different internal couplings \mathcal{I} samples (indexed by $0 \leq i < \mathcal{N}_{\mathcal{I}}$) and, for each of these, we use $\mathcal{N}_{\mathcal{O}} = 1280$ different outer disorder \mathcal{O} realizations (indexed by $0 \leq o < \mathcal{N}_{\mathcal{O}}$). Thus we have a total of $\mathcal{N}_{\mathcal{J}} = 12800$ samples and, for each sample $\mathcal{J} = \mathcal{I}\mathcal{U}\mathcal{O}$, we simulate $m = 4$ distinct real replicas.

We take $\mathcal{N}_{\mathcal{I}} \ll \mathcal{N}_{\mathcal{O}}$ because we expect all inner disorder samples to be “typical” [9] when computing metastate averages at $R \gg 1$. We found however sizable sample-to-sample fluctuations for the system sizes we consider.

The average over the Gibbs state $\langle \dots \rangle_{\Gamma}$ is estimated via Monte Carlo thermal averages $\langle \dots \rangle$ at fixed disorder \mathcal{J} , i.e., for given indices i and o . The average over the metastate is given by $[\dots]_{\kappa} = \sum_o (\dots) / \mathcal{N}_{\mathcal{O}}$, and the one over the internal disorder by $(\dots) = \sum_i (\dots) / \mathcal{N}_{\mathcal{I}}$. For example, the MAS spin correlation function is given by

$$C_{\rho}(x) = \overline{[\langle s_0 s_x \rangle_{\Gamma}]_{\kappa}^2} = \frac{1}{\mathcal{N}_{\mathcal{I}}} \sum_i \left(\frac{1}{\mathcal{N}_{\mathcal{O}}} \sum_o \langle s_0^{i;o} s_x^{i;o} \rangle \right)^2 \\ = \frac{1}{\mathcal{N}_{\mathcal{I}}} \sum_i \frac{1}{\mathcal{N}_{\mathcal{O}}^2} \sum_{o,o'} \langle s_0^{i;o} s_x^{i;o} s_0^{i;o'} s_x^{i;o'} \rangle \sim |x|^{-(d-\zeta)}, \quad (2)$$

defining Read’s ζ exponent for $|x| \gg 1$.

We measure in Λ_W the overlaps between any two real replicas, let us call them $\underline{\sigma}$ and $\underline{\tau}$, sharing the same internal disorder (indexed by i) and having external couplings indexed by o and o' ,

$$q_{i;o,o'} \equiv \frac{1}{W^3} \sum_{x \in \Lambda_W} \sigma_x^{i;o} \tau_x^{i;o'}. \quad (3)$$

Actually, for each $\{i; o, o'\}$, we have $m(m-1)/2$ contributions from different pairs of real replicas if $o = o'$ and m^2 otherwise.

The main objects of our numerical study are the probability density functions (PDF) of the overlaps,

$$P(q) = \frac{\sum_i P_i(q)}{\mathcal{N}_{\mathcal{I}}}, \quad P_i(q) = \frac{1}{\mathcal{N}_{\mathcal{O}}} \sum_o \langle \delta(q - q_{i;o,o}) \rangle, \\ P_{\rho}(q) = \frac{\sum_i P_{\rho,i}(q)}{\mathcal{N}_{\mathcal{I}}}, \quad P_{\rho,i}(q) = \frac{1}{\mathcal{N}_{\mathcal{O}}^2} \sum_{o,o'} \langle \delta(q - q_{i;o,o'}) \rangle.$$

While $P(q)$ is the usual PDF already measured in many numerical simulation of spin glasses, $P_{\rho}(q)$ is the PDF of the overlap over the MAS. Although $P_{\rho}(q) \rightarrow \delta(q)$ for $W \rightarrow \infty$ [9], the scaling of its variance is informative,

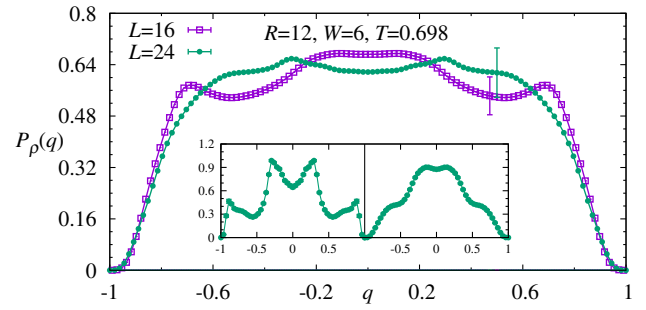


FIG. 2. Main plot: The MAS overlap distribution $P_{\rho}(q)$ with $R = 12$ at $T = 0.698 \approx 0.64T_c$ shows no statistical significant dependence on the lattice size L (the error bars, computed from fluctuations on \mathcal{I} , are shown for one value of q only for the sake of clarity). Inset: $P_{\rho,i}(q)$ for two specific configurations of the inner disorder \mathcal{I} (the error bars, computed from fluctuations on \mathcal{O} , are smaller than the data points).

$$\chi_{\rho} = \sum_{x \in \Lambda_W} C_{\rho}(x) = W^d \int q^2 P_{\rho}(q) dq \sim W^{\zeta}. \quad (4)$$

Numerical results.—Taking the limit of large L in simulations actually amounts to asking how small the ratios R/L and W/R need to be, in order to find results that are safe (to a given accuracy).

In Fig. 2 (main plot) we see that the MAS $P_{\rho}(q)$ measured with $R = 12$ and both $L = 24$ and $L = 16$ are statistically compatible, suggesting that $R/L = 3/4$ is already a safe choice. The error bars are rather large, because the dependence of $P_{\rho,i}(q)$ on the internal disorder sample is unexpectedly strong for the values of W and R we are using (as shown by the insets in Fig. 2).

A similar check can be performed with the MAS susceptibility χ_{ρ} (see Fig. 3). In the inset we see that, fixing $R = 12$, all data with $R/L \leq 3/4$ are statistical compatible, while data with $R/L = 6/7$ show significant deviations even for small W values. Hereafter we safely fix $R = L/2$.

The main panel of Fig. 3 shows data for the MAS susceptibility χ_{ρ} measured with the safe ratio $R = L/2$

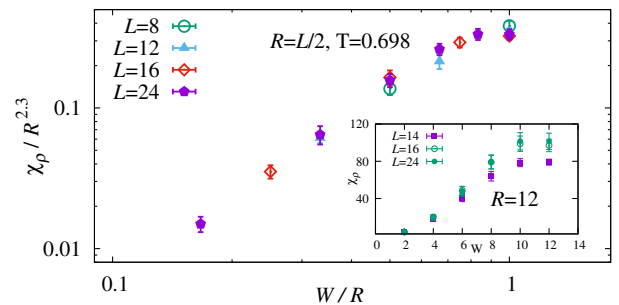


FIG. 3. Main plot: Collapse of MAS susceptibility data measured with $R = L/2$ at $T = 0.698 \approx 0.64T_c$. Inset: Deviations from the asymptotic behavior are evident only for $R/L > 3/4$.

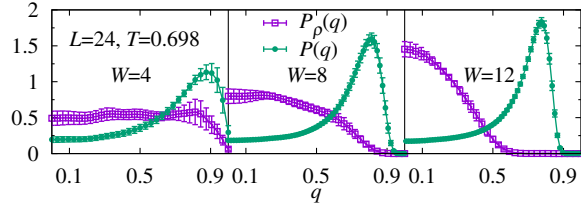


FIG. 4. $P_\rho(q)$ and $P(q)$ for $L = 24$, $R = L/2$, and $T = 0.698$ and different values of the measuring window size, $W = 4, 8, 12$.

(which is statistically equivalent to the limiting condition $R \ll L$) and different ratios W/R . Data have been rescaled according to the following scaling law,

$$\chi_\rho(W, R) = R^\zeta f(W/R) = W^\zeta g(W/R), \quad (5)$$

which is compatible with Eq. (4) if $f(x) \propto x^\zeta$ for $x \ll 1$ and $g(0) = \text{const}$. First of all we note that the physical behavior we would like to measure in the limit $W/R \ll 1$ actually extends up to $W/R \approx 0.75$, where corrections to the asymptotic power law appear. Fitting data with $W/R < 0.75$ we estimate Read's exponent $\zeta = 2.3 \pm 0.3$ (we have not found any evidence of size corrections in the computation of ζ [39]).

Finally we show in Fig. 4 the size dependence of both $P_\rho(q)$ and $P(q)$, for $L = 24$ (the largest simulated), $R = L/2$, and varying W . For a dispersed metastate in the thermodynamic limit the two distributions are different.

Discussion and conclusions.—We have shown that state-of-the-art numerical simulations of spin glasses in $d = 3$ allow for the construction of the AW metastate. Numerical data suggest that the limiting conditions $1 \ll W \ll R \ll L$ can be relaxed to $W/R, R/L \approx 3/4$ without changing substantially the thermodynamic physical behavior. This is unexpected very good news.

From the numerical construction of the AW metastate we have obtained quantitative information on the nature of the spin-glass phase in $d = 3$. The metastate average overlap distribution $P(q)$ and the MAS $P_\rho(q)$ are significantly distinct objects already at moderate sizes. We cannot extrapolate safely to the thermodynamic limit, and sample-to-sample fluctuations are still important at the accessible system sizes. Nevertheless we have found a convincing scaling law for the MAS susceptibility, and an estimate of $\zeta(d = 3) = 2.3(3)$, strongly suggesting $\zeta < d$.

Read's exponent ζ is related to the number of different states that can be measured in a system of size W as $\log n_{\text{states}} \sim W^{d-\zeta}$ [9]. Such a number diverges in the thermodynamic limit as long as $\zeta < d$, supporting the picture of a metastate with infinitely many states. In Fig. 5 we summarize our knowledge about the ζ exponent. At and above the upper critical dimension $d_U = 6$, where mean field exponents are correct, $\zeta = 4$ [44,45]. Assuming $\zeta(d)$ is a continuous and monotonically nondecreasing function, the inequality $\zeta < d$ still holds slightly below d_U .

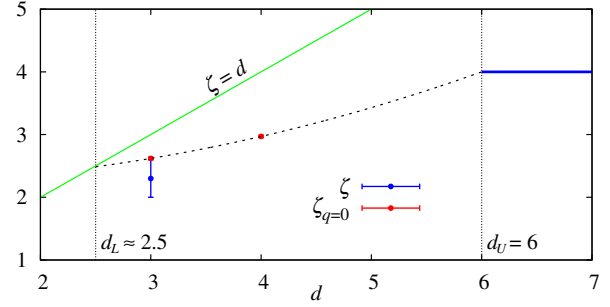


FIG. 5. The exponent ζ as a function of d .

In the present work we find $\zeta(d = 3) = 2.3(3)$ (blue point in Fig. 5). An alternative estimate of the ζ exponent comes from the decay of the four-spins spatial correlation function conditional to the $q = 0$ sector, $C_4(x) = \overline{[\langle \sigma_0^{i;o} \tau_0^{i;o} \sigma_x^{i;o} \tau_x^{i;o} \rangle_{\Gamma|q_{i;o,o}=0}]_\kappa} \sim |x|^{-(d-\zeta_{q=0})}$ for $|x| \gg 1$: $\zeta_{q=0}(d = 3) = 2.62(2)$ [36,46,47] and $\zeta_{q=0}(d = 4) = 2.97(2)$ [48]. Read conjectured that $\zeta_{q=0} = \zeta$ [9]. These estimates are shown by red points in Fig. 5 [49]. A gentle interpolation of the ζ estimates (dashed line in Fig. 5) seems to meet the $\zeta = d$ condition very close to the current best estimate for the lower critical dimension $d_L \approx 2.5$ [50].

In conclusion, all the numerical evidences strongly support the existence of a spin-glass metastate dispersed over infinitely many states for $d = 3$ (and probably down to the lower critical dimension). These findings are incompatible with the droplet model, while they are compatible with both the chaotic pair picture and the replica symmetry breaking scenario.

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