# Nature of Ergodicity Breaking in Ising Spin Glasses as Revealed by Correlation Function Spectral Properties

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In this Letter we address the nature of broken ergodicity in the low temperature phase of Ising spin glasses by examining spectral properties of spin correlation functions $C_{ij} \equiv \langle S_i S_j \rangle$. We argue that more than one extensive [i.e., $O(N)$] eigenvalue in this matrix signals replica symmetry breaking. Monte Carlo simulations of the infinite-range Ising spin-glass model, above and below the Almeida-Thouless line, support this conclusion. Exchange Monte Carlo simulations for the short-range model in four dimensions find a single extensive eigenvalue and a large subdominant eigenvalue consistent with droplet model expectations.

Following Parisi's [1] demonstration of replica symmetry breaking in the low-temperature phase of the Sherrington-Kirkpatrick (SK) model [2], there has been an ongoing debate concerning the nature of the low-temperature phase of Ising spin glasses in finite dimensions, and of glassy states in quenched-disorder systems more generally. The Parisi solution breaks ergodicity through the segregation of phase space into many ergodic regions, separated by energy barriers which are infinite in the limit $N \rightarrow \infty$ (where $N$ is the number of spins). Each of these regions, in the case of a Hamiltonian invariant under global spin inversion, has an associated region related to it by global spin inversion, the pair forming together what we will refer to as a pure state pair (PSP) [3]. In the low-temperature phase of the SK model, there are many PSP's, unrelated by any symmetry of the Hamiltonian. In accord with common usage we will call this form of ergodicity breaking "replica symmetry breaking" or RSB [4]. While the Parisi solution shows every sign of being correct for the infinite-range (hence infinite-dimension) SK problem, there is still no consensus on the form of ergodicity breaking in models with finite-range interactions. An alternative to the RSB scenario is the "droplet" picture [5], which postulates a single PSP in the low-temperature phase, whose excitations include rare large droplets of overturned spins with energy (at size $L$) scaling as $L^{\theta}$.

The principal numerical tool for detecting replica symmetry breaking has been finite size scaling of the probability distribution function $P(q)$ for the overlap $q$ between the local magnetizations in different pure states. Several numerical studies have suggested a behavior in finite dimensions similar to the one at the mean field level [6,7]. Other studies using the Migdal-Kadanoff approximation [8] and still others at zero temperature [9] have suggested otherwise and favor the droplet model. None of these studies has conclusively resolved which type of broken ergodicity takes place in the low-temperature phase in finite dimension, motivating a search for new approaches.

We suggest that the nature of the low-temperature phase can be determined by studying the spectrum of the spin-spin correlation function $\langle S_i S_j \rangle \equiv C_{ij}$. In the case of a single PSP we will argue that this correlation function has at most a single extensive eigenvalue. Thus, we take the existence of more than one extensive eigenvalue to be clear evidence for multiple PSPs, i.e., RSB. Our main results are shown in Fig. 1, where we illustrate this behavior using exchange Monte Carlo (MC) [10] simulations for the SK model, both above (where there is a single pure state) and below the Almeida-Thouless (AT) line [11]. We have also used MC simulations to study Ising spin glasses in four dimensions. Here we see no signs of RSB out to the largest size studied ($N = 6^4$ spins) and instead find finite size behavior for the second largest eigenvalue which is consistent with droplet model expectations.

At a continuous symmetry-breaking phase transition, a suitably defined correlation function develops long-range order. In systems without quenched disorder, the eigenvalues $C(\vec{k})$ of the appropriate correlation function can typically be labeled by wave vector $\vec{k}$, and the long-range order is signaled by $C(\vec{k})$ becoming extensive below the transition temperature at a single value of $\vec{k}$. In systems with quenched disorder, the correlation function eigenfunctions are not plane waves, but long-range order is still signaled by an extensive eigenvalue. For Ising spin glasses, the correlation function matrix $C_{ij}$ is a real symmetric positive semidefinite matrix with trace equal to the number of sites $N$, and is analogous to the one-particle density matrix of a superfluid. In either system the order is off-diagonal in a position basis, and the fact that it is long ranged is reflected in its spectrum: an extensive eigenvalue always signals long-range order since the associated eigenfunction must be extended [12].

We now argue that there will be only one extensive eigenvalue in the case of broken ergodicity with a single PSP. We rewrite
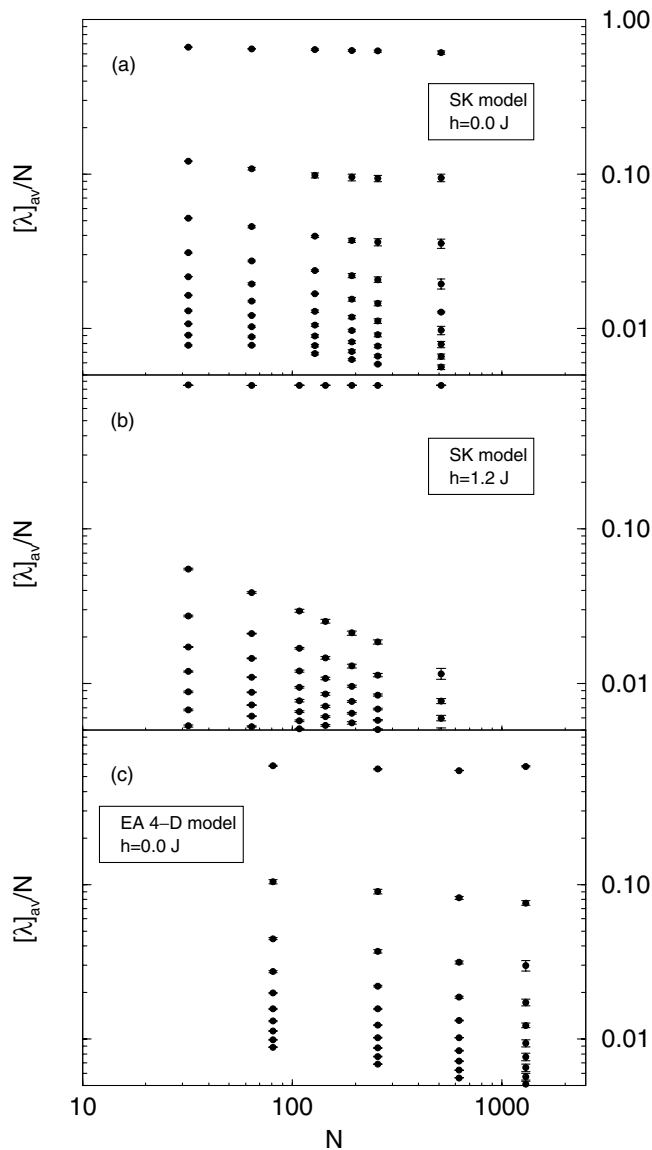
FIG. 1. Scaling of the average of the ten largest eigenvalues of $C_{ij}$ as a function of system size $N$ in (a) the SK model below the AT line ($h = 0$, $T/J = 0.4$), (b) the SK model above the AT line ($h/J = 1.2$, $T/J = 0.4$), and (c) the EA model in 4D ($h/J = 0$, $T/J = 1.0$).

$$C_{ij} = \langle S_i \rangle \langle S_j \rangle + V_{ij}, \qquad (1)$$

where $V_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle = \langle S_i S_j \rangle_c$ is the connected correlation function. If we ignore $V$, the matrix $C_{ij}$ is a pure projector $C^0 \equiv |v\rangle\langle v|$ onto the state $|v\rangle$ with $v_i = \langle S_i \rangle$. $C^0$ has one large eigenvalue $\langle v|v \rangle = \mathrm{Tr}C^0 = \sum_i \langle S_i \rangle^2$, and the remaining eigenvalues are zero. The influence of $V$ on the spectrum of $C_{ij}$ depends on the typical value of its matrix elements. If we assume that $V_{ij} \sim N^{-\delta}$ with $\delta > 0$, it follows from first order perturbation theory that the largest eigenvalue will still be extensive,

and that the largest subdominant eigenvalue $\lambda_2 \sim N^{1-\delta}$ at most.

In some cases we can put a bound on $\delta$. For instance, if we simply assume that the spin-glass susceptibility $\chi_{SG}$ is of $O(1)$, then we get $\delta \geq 1/2$. This should be the case above the AT line in the SK model. The calculations shown in Fig. 1(b) conform to this picture, with $\delta$ changing smoothly from $\sim 1/2$ in the figure to $\sim 1$ for larger $h$ (where the correlations approach those of a ferromagnet, and hence $\delta \to 1$).

While the above arguments make no direct reference to spatial dimension, they do rely on the notion of a "typical" element of $V$. This idea is certainly appropriate for infinite-range models such as the SK problem. We are, of course, most interested in finite-dimensional problems with a spin-glass phase above zero temperature. Here the outstanding alternative to the many-valley picture is the droplet picture [5]. In this picture there are typical elements of $V$ which are exponentially small, plus a set of elements of $O(1)$ in magnitude. The fraction of the latter is of $O(1/L^\theta)$ where $L$ is the system size and $\theta$ is a scaling exponent from the zero-temperature fixed point. Again we consider the "worst" case: supposing that $V$ for a finite sample is dominated by one large active droplet of the size of $O(L)$, then the big elements of $V$, appearing with probability $\sim 1/L^\theta = 1/N^{\theta/d}$, are coherent, and so will give a large eigenvalue of order $N \times N^{-\theta/d} = N^{1-\theta/d}$. (We have verified this with simple numerical experiments.) If $V$ is incoherent then its eigenvalues should grow more slowly (or decay) with $N$. Hence, given the principal scaling assumption of the droplet picture, we expect the second eigenvalue $\lambda_2$ of $C_{ij}$ to grow as $N^{1-\theta/d}$ or slower.

It follows from the above arguments that as long as there is one PSP (or one pure state), there can be no more than one eigenvalue of $C$ which is of order $N$. Thus the observation of more than one such eigenvalue directly implies multiple PSPs, i.e., RSB.

The SK model is a perfect candidate to test our ideas regarding multiple large eigenvalues of $C_{ij}$, since we can tune the nature of the broken ergodicity by simply varying the external magnetic field $h$. We have performed numerical calculations using exchange MC [10], which allows for faster jumps across large energy barriers. Our criteria for equilibration follow closely those used in Ref. [7]. We check for agreement between two different ways of calculating $\chi_{SG}$; one method [13,14] uses the averaging of the overlap of two uncoupled replicas, and the other uses the standard thermal averaging in MC simulations. We also check the symmetry of $P(q)$ and the variance of the eigenvalues of $C_{ij}$.

We find that the probability distributions of the eigenvalues of $C$ are broad (at least for the first two eigenvalues) below the AT line, and very sharp above it. We illustrate this in Fig. 2. The breadth of these distributions indicates the need to do disorder averaging over a large ensemble (300–2000), at least in the spin-glass phase. In
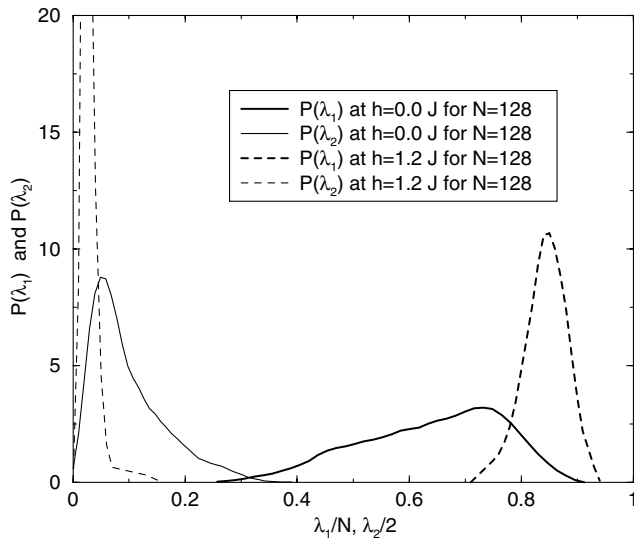
FIG. 2. Distribution of the first (thick lines) and second (thin lines) eigenvalue of $C_{ij}$ in the SK model at $h/J = 0$ (solid line) and $h/J = 1.2$ (dashed line), above the AT line. Here $T/J = 0.4$ and $N = 128$.

Fig. 1 we show the scaling of the disorder average of the ten largest eigenvalues as a function of system size, both below [Fig. 1(a)] and above [Fig. 1(b)] the AT line in the SK model. It is clear from Fig. 1(a) that at least two eigenvalues are of $O(N)$ for $N \gtrsim 100$. We expect [15] further $O(N)$ eigenvalues to emerge for larger $N$, as suggested by the behavior of $[\lambda_3]_{av}$ in the figure. In contrast, there is only one large eigenvalue in Fig. 1(b). We find further that, above the AT line, $[\lambda_2]_{av}/N \sim N^{-0.52}$, consistent with our previous arguments. MC results for larger $h$ show that $[\lambda_2]_{av}/N$ decays with a larger exponent (we have observed up to $\sim 0.75$), which we expect to approach 1 for large enough $h$.

Figure 1(a) suggests that the spectrum of $C_{ij}$ for the SK problem is dominated by two large eigenvalues (for the sizes considered here). We can reproduce this behavior with the following simple model. Suppose that phase space consists of only two spin configurations 1 and 2, and ignore all others. Take $C(\alpha) = \alpha C^{(1)} + (1 - \alpha)C^{(2)}$, with $C^{(1)}$ and $C^{(2)}$ corresponding to the $C_{ij}$ of the two different configurations $S_i^{(1)}$ and $S_i^{(2)}$ at zero $T$, and $\alpha$ (a thermodynamic weight) ranging from 0 to $1/2$. The overlap between the two states is given by $q_{12} = \sum_i S_i^{(1)} S_i^{(2)}/N$. It can easily be shown that this matrix has only two nonzero eigenvalues, corresponding to

$$\frac{\lambda_{\pm}(q_{12}, \alpha)}{N} = \frac{1 \pm \sqrt{q_{12}^2 + (1 - q_{12}^2)(2\alpha - 1)^2}}{2}. \tag{2}$$

Note that $\lambda_{\pm}/N$ range from 1 and 0 at $\alpha = 0$ to $(1 \pm |q_{12}|)/2$ at $\alpha = 1/2$. It is clear from (2) that the two largest

eigenvalues can vary over a wide range, while still in general remaining of $O(N)$ [16]. Hence (as we saw numerically) it is important to study the probability distribution for each eigenvalue $\tilde{P}(\lambda_i)$, rather than the distribution of the eigenvalues for a single disorder realization. At this low level of approximation we already see that the probability distributions of the first two eigenvalues will be very broad in the frozen phase whenever the probability distribution of $q_{12}$, $P_{12}(q)$, is broad. This simple picture, however, lacks any finite temperature and correlation effects. To introduce temperature in the model we let $S_i^{(1)}$ and $S_i^{(2)}$ become Gaussian random variables. We decompose $P(q)$ from our MC data as $(1/2)[P_{11}(q) + P_{12}(q)]$, with $P_{11}(q)$ (the self-overlap) a Gaussian which determines the mean and variance of $S_i^{(1)}$ and $S_i^{(2)}$. We then adjust their relative distribution to match $P_{12}(q)$. This gives us a joint distribution for $S_i^{(1)}$ and $S_i^{(2)}$ which we use to generate a distribution of matrices $C(\alpha = 1/2)$. The eigenvalues may then be obtained either by an analytical perturbation approach or by direct numerical diagonalization of the matrix $C$. Figure 3 compares the resulting eigenvalue distributions for $N = 64$, with those obtained directly from the MC results for the SK model. It is striking how closely they resemble one another in qualitative and quantitative behavior, given the simplicity of our two-state model.

Thus we find a clear confirmation of our ideas in the behavior of the SK model, for which we know the nature of the ergodicity breaking in the various equilibrium phases. We now use these ideas to study the four-dimensional Ising spin glass or Edward-Anderson (EA) model, with nearest-neighbor interactions and a Gaussian distribution of the $J_{ij}$'s with variance $J$. In Fig. 1(c) we show the scaling of $[\lambda_i]_{av}/N$ for the first ten eigenvalues of $C$ at $T/J = 1.0$
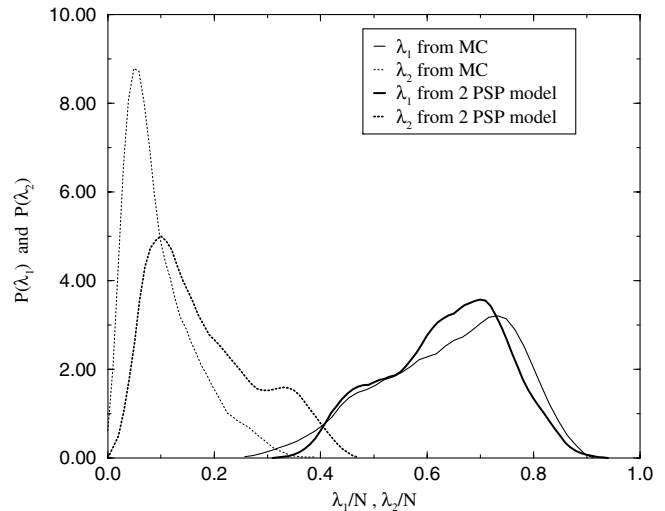


FIG. 3. Distribution of the first (solid line) and second (dashed line) eigenvalue of $C_{ij}$ obtained from the MC simulation of the SK model at $N = 64$ and $T/J = 0.4$ (thin line), and the respective distributions obtained from the two pure state model simulation (thick line) with $\alpha = 1/2$.

and $h/J = 0$. These runs are rather deep into the frozen phase, since [17] $T_c \approx 1.75J$. We choose this low temperature in order to work as far as possible from the critical region. This low temperature, plus the time involved in measuring $C_{ij}$, has limited us thus far to $L \leq 6$. (We note that, even at this low temperature, we are still not fully out of the critical region, according to Ref. [18].) In this region of size and temperature we find, as in the SK spin glass phase, a broad and asymmetric distribution of $\lambda_1$ and $\lambda_2$, similar to that for the frozen phase illustrated in Fig. 2.

We have studied both $[\lambda_i]_{av}$ and $(\lambda_i)_{typ}$ for these distributions [the latter defined as $\exp([\ln \lambda_i]_{av})$]. Figure 1(c) shows $[\lambda_2]_{av}/N$ decaying with $N$. On a double-log scale we see a clear straight line with exponent $\sim 0.11$. The behavior for $(\lambda_2)_{typ}$ is similar, except the exponent is larger, $\sim 0.15$. This latter exponent is consistent with our lower bound for $\delta$, given that estimates of $\theta$ in 4D range [10,19] from 0.6 to 0.8. Hence these data appear to fit the droplet scenario, with a single PSP in the frozen phase. We cannot, of course, rule out the possibility that the $[\lambda_2]_{av}/N$ points (and others for $i > 2$) may flatten out at larger $N$, as occurred for the SK case at about $N = 100$. Only further work at larger $N$ can help with this question. Also, while it is consistent that $(\lambda_2)_{typ}/N$ decays as expected according to our arguments and the droplet picture, the slower decay of $[\lambda_2]_{av}/N$—which clearly results from the skew in the distribution—needs some understanding.

In summary, we have proposed, and numerically tested, a new method for identifying the nature of ergodicity breaking in RSB in Ising spin glasses. We believe [15,16] that RSB occurs if and only if the spin correlation function has multiple large eigenvalues. Our MC results for the infinite-range SK problem show a clear qualitative difference in the long-range order above and below the AT line. Because of the generality of these ideas, we expect that they may be applied to other quenched disorder problems in statistical physics for which RSB is a possibility. We have also presented results for the EA model in four space dimensions. Because of the finite-size effects plaguing all spin-glass simulations, these results cannot be viewed as conclusive. However, our results over the entire range for which we can reliably compute both thermal and disorder averages tend to support the droplet picture, with one pure-state pair: we see no sign of multiple large eigenvalues, and $(\lambda_2)_{typ}/N$ decays roughly in line with droplet model expectations. Future work based on this approach should shed significant further light on the nature of ergodicity breaking in finite-dimensional spin glasses.

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