

Multiple states and thermodynamic limits in short-ranged Ising spin-glass models

C. M. Newman

Courant Institute of Mathematical Sciences, 251 Mercer Street, New York, New York 10012

D. L. Stein

Department of Physics, University of Arizona, Tucson, Arizona 85721

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We propose a test to distinguish, both numerically and theoretically, between the two competing pictures of short-ranged Ising spin glasses at low temperature: "chaotic" size dependence. Scaling theories in which at most two pure states (related by a global spin flip) occur require that finite-volume correlations (with, say, periodic boundary conditions) have a well-defined thermodynamic limit. We argue, however, that the picture based on the infinite-ranged Sherrington-Kirkpatrick model, with many non-congruent pure states, leads to a breakdown of the thermodynamic limit. The argument combines rigorous and heuristic elements; one of the former is a proof that in the infinite-ranged model itself, non-self-averaging implies chaotic size dependence. Numerical tests, based on chaotic size dependence, could provide a more sensitive measure than the usual overlap distribution $P(q)$ in determining the number of pure states.

I. INTRODUCTION

The question of multiplicity of pure states in the Edwards-Anderson (EA) short-ranged Ising spin glass model¹ remains open despite intensive study over a decade and a half.² The Parisi solution³ of the infinite-ranged Sherrington-Kirkpatrick (SK) model⁴ indicates the existence of many distinct states at low temperature and field. For the short-ranged model there presently exist primarily two opposing points of view. Scaling theories⁵⁻⁷ suggest that, unlike the infinite-ranged model, no more than two pure states exist at any temperature and field.^{8,9} Others have argued, by analogy with the SK model, that short-ranged models in sufficiently high dimension should exhibit many pure states (see, for example, Ref. 2) for some range of temperatures and fields.

In most of these papers, what is actually meant by "multiplicity of states" is not made precise, a notable exception being Ref. 8. The standard procedure for generating a thermodynamic state is to choose a set of boundary conditions on a sequence of volumes increasing to infinity; for each volume, one computes all thermodynamic quantities and correlation functions using the standard Gibbs prescription, and the limiting values (if they exist) of all the correlations specify a thermodynamic state.¹⁰ This state may be a *pure* state, meaning that it cannot be expressed as a convex combination of other Gibbs states; or it may be a *mixed* state, such as that produced in the Ising ferromagnet below T_c from an infinite sequence of periodic boundary conditions. In that case, the state produced consists of a sum of two pure translation-invariant states, the "plus" state with a majority of bulk spins up and the "minus" state with the majority down, each with probability $\frac{1}{2}$.

In the case of the spin-glass model described below, let us consider, as in recent numerical studies,^{11,12} a sequence of cubes Λ_L (of length scale L , centered at the ori-

gin) with periodic boundary conditions. Those studies evaluate numerically a function $P(q)$, the order parameter distribution, and find a continuous portion extending down to $q=0$, as in the SK model.¹³ Although at first glance this seems to support the SK picture, this is not unambiguously so: finite-volume effects could create a continuous portion of $P(q)$ even if the limiting thermodynamic state were a mixture of only two pure states,⁸ as predicted by the scaling picture. It seems implicit in the discussions of Refs. 11 and 12 that the more likely alternative to the above possibility is the existence of a limiting thermodynamic state ρ which is a mixture of (countably) many pure states ρ^α , with weights W_α ; the ρ^α 's and W_α 's would be non-self-averaging, i.e., would depend on the couplings in such a way that an average over couplings would yield the continuous portion of $P(q)$. The question of whether there exists a thermodynamic limit at all has not been discussed.

In this paper we argue that the actual situation in simple nearest-neighbor Ising spin-glass models is more subtle than previously suspected, and that this subtlety can be exploited to yield an unambiguous test that distinguishes between the scaling and SK pictures.¹⁴ We will show that the problem of existence of many pure Gibbs states in spin glasses is sensitively tied to the question of whether an infinite sequence of coupling-independent boundary conditions, such as periodic, possesses an infinite-volume limit. Indeed, we claim that this is actually the crux of the problem of multiplicity of states.

We will argue, through a combination of rigorous proof and heuristic argument, that the SK picture leads to a situation in which the infinite-volume limit does not exist; i.e., one in which to obtain a thermodynamic state it is necessary to choose a (coupling dependent) subsequence of L 's, such that different subsequences yield different thermodynamic states for a single coupling configuration. *Thus, in addition to non-self-averaging due*

to coupling dependence for fixed size, the SK picture seems to require some kind of chaotic size dependence for fixed coupling. If such chaotic size dependence does not occur, it would follow by our arguments that the SK picture is invalid (or else, to paraphrase Ref. 12, it is missing some important ingredient). On the other hand, if chaotic size dependence does occur, it easily follows that the scaling picture is invalid. We emphasize that the test we propose is based on a chaotic size dependence of the state (or equivalently, of the correlation functions), and not of thermodynamic functions like the free energy per spin, which should always have a well-defined (and self-averaged) thermodynamic limit.

The details of our arguments, which contain both rigorous proofs and heuristic analysis, are presented in the next two sections; we briefly sketch them now. First, we prove (Theorem 2), by a simple and standard argument, that the scaling picture forbids chaotic size dependence; i.e., it implies the existence of a thermodynamic limit for the state. Next, as a first step in showing the inconsistency of the SK picture with existence of a thermodynamic limit, we prove (Theorem 3) that if a thermodynamic limit for the state exists with (say) periodic boundary conditions, then it also exists with any other flip-related boundary condition (e.g., antiperiodic) and the two thermodynamic states obtained must be identical. That is, the two states are of the form $\sum_{\alpha} W_{\alpha} \rho^{\alpha}$, with the same pure states ρ^{α} and the same weights W_{α} . We end Sec. II with heuristic arguments, for both zero and nonzero temperatures, which suggest that in the SK picture, periodic and antiperiodic boundary conditions should not yield identical ρ^{α} 's and W_{α} 's.

Although chaotic size dependence may at first seem unnatural, we show in Sec. III by several examples that in fact it is rather typical in disordered systems. The first, and most important, example is the infinite-ranged SK model itself. Here we consider $P_N^{\mathcal{J}}(q)$, the N -spin order parameter distribution for fixed couplings (denoted by \mathcal{J}). More precisely, $P_N^{\mathcal{J}}(q)$ is the distribution of the overlap sum between the original N -spin system and a duplicate [see Eq. (11) in Sec. III]; it is often expressed, somewhat imprecisely, as the distribution of the overlaps $q_{\alpha\beta}^{\mathcal{J}}$ among states:

$$q_{\alpha\beta}^{\mathcal{J}} = (1/N) \sum_{i=1}^N \langle S_i \rangle^{\alpha} \langle S_i \rangle^{\beta}. \quad (1)$$

The usual interpretation¹⁵ of the Parisi solution suggests that, as $N \rightarrow \infty$, $P_N^{\mathcal{J}}(q)$ converges to a countable sum of δ functions,

$$\sum_{\alpha, \beta} W_{\alpha}^{\mathcal{J}} W_{\beta}^{\mathcal{J}} \delta(q - q_{\alpha\beta}^{\mathcal{J}}) \quad (2)$$

which, after averaging over the couplings, yields $P(q)$ with a continuous portion, as discussed above. In other words, non-self-averaging is taken to mean existence of a coupling-dependent limit for $P_N^{\mathcal{J}}(q)$. This cannot be so: we prove that, if the $N \rightarrow \infty$ limit exists before averaging over the couplings, then that limit must already be self-averaged. Therefore, if there is indeed non-self-averaging, as predicted by the Parisi solution,¹⁵ then

there must be chaotic N dependence [of $P_N^{\mathcal{J}}(q)$] for fixed couplings. We therefore argue that an SK picture for short-ranged models with chaotic size dependence is most consistent with the situation in the infinite-ranged model.

Section III concludes with four more examples of chaotic size dependence: (i) the zero-temperature spin glass with a fixed configuration; (ii) an *ad hoc* two-dimensional model with random couplings only along a one-dimensional line; (iii) the Ising ferromagnet in a random field; and (iv) the Ising ferromagnet with random boundary conditions.

In Sec. IV we discuss various refinements of the scaling picture and related issues such as a possible weak uniqueness of the thermodynamic state. We discuss here questions of volume dependence of free energy differences among noncongruent pure states, and their relation to the Fisher-Huse¹⁶ inequality for the scaling exponent, $\theta \leq (d-1)/2$. In Sec. V, we discuss refinements of the SK picture including such issues as whether there need be coexistence of pure phases at all in "typical" large volumes. We then use these results to discuss in more detail how a numerical test for chaotic size dependence could be conducted.

II. THERMODYNAMIC LIMITS

We will henceforth consider the d -dimensional Ising spin glass described by the EA Hamiltonian:¹

$$\mathcal{H} = - \sum_{ij} J_{ij} S_i S_j, \quad (3)$$

where $i \in \mathbb{Z}^d$, $S_i = \pm 1$, and the angular brackets under the summation sign indicate a sum over nearest-neighbor pairs only. The couplings J_{ij} are chosen with quenched, independent randomness with a common distribution. Usually (as indicated) we will assume that the distribution is symmetric and sometimes that it is continuous. For definiteness, one may use a Gaussian distribution of mean zero and variance one; i.e., one with probability density

$$\frac{1}{\sqrt{2\pi}} e^{-J_{ij}^2/2}. \quad (4)$$

We will denote by \mathcal{J} a configuration of all the J_{ij} 's for all $\langle ij \rangle$ in \mathbb{Z}^d .

For each $L = 1, 2, 3, \dots$, let Λ_L denote the cube¹⁷ $\{-L+1, -L+2, \dots, L\}^d$ in \mathbb{Z}^d , let ρ_L denote the finite volume Gibbs distribution on the spin configurations in Λ_L at some fixed temperature T with some boundary condition chosen for each L , and let $\langle \cdot \rangle_L$ denote the thermal average with respect to ρ_L . We are primarily interested in \mathcal{J} -independent boundary conditions; i.e., ones in which the boundary conditions may depend on L but not \mathcal{J} . We will say, for a given \mathcal{J} , that ρ_L has an infinite-volume limit if for each m and for each i_1, \dots, i_m in \mathbb{Z}^d ,

$$\langle S_{i_1} \cdots S_{i_m} \rangle \equiv \lim_{L \rightarrow \infty} \langle S_{i_1} \cdots S_{i_m} \rangle_L \text{ exists.} \quad (5)$$

We will then also write $\rho_L \rightarrow \rho$ where ρ is the (infinite volume) Gibbs distribution all of whose correlations are given by (5). We now state a standard fact about such infinite-volume limits in disordered systems at nonzero

temperatures.¹⁸

Theorem 1. If the boundary conditions are \mathcal{J} independent, then either ρ_L has an infinite-volume limit for almost all \mathcal{J} or else ρ_L does not have an infinite-volume limit for almost all \mathcal{J} . (Almost all means except for a set of \mathcal{J} 's with zero probability in the ensemble of \mathcal{J} 's.)

Proof. Suppose \mathcal{J} is a configuration of couplings for which $\rho_L^{\mathcal{J}}$ has an infinite-volume limit, and suppose \mathcal{J}' differs from \mathcal{J} only for finitely many J_{ij} 's. It is easy to see by explicit calculation that the finite-volume correlations of $\rho_L^{\mathcal{J}'}$ can be expressed as specific L -independent functions of the correlations for \mathcal{J} and thus $\rho_L^{\mathcal{J}'}$ must also have an infinite-volume limit. Thus, by the Kolmogorov zero-one law,¹⁹ the set of \mathcal{J} 's for which there exists an infinite-volume limit of $\rho_L^{\mathcal{J}}$ (as an event which does not depend on any finite number of couplings) either has probability zero or probability one.

For a given \mathcal{J} , the set of all Gibbs states is the set of all the ρ 's which arise by the limit (5) for some (possibly \mathcal{J} -dependent) choice of boundary conditions. As mentioned previously, a Gibbs state is pure if it is not a mixture of other Gibbs states (for the same \mathcal{J}).

It is a standard result,²⁰ whose proof is quite similar to Theorem 1, that the number of pure Gibbs states is the same for coupling configurations \mathcal{J} and \mathcal{J}' which differ only for finitely many J_{ij} 's and thus this number takes some fixed value (1 or 2 or . . . or ∞) for almost all \mathcal{J} . According to the scaling picture, at low temperature there are (for almost all \mathcal{J}) exactly two pure Gibbs states, which transform into each other via a global spin flip.

The next theorem shows that chaotic L dependence cannot happen in the scaling picture for symmetric (i.e., flip-invariant) choices of boundary conditions; its proof is simple and standard.²¹ We will call boundary conditions symmetric if for each L , ρ_L is invariant under a flip of all the spins in Λ_L ; i.e., all odd order correlations of spins in Λ_L vanish. Examples of symmetric boundary conditions are periodic, antiperiodic, and mixtures of fixed boundary conditions in which each boundary spin configuration appears with the same weight as its flip. This theorem allows \mathcal{J} -dependent boundary conditions.

Theorem 2. Let \mathcal{J} be fixed. Assume that there are exactly two pure Gibbs states, ρ^+ and ρ^- , and that these transform into each other under a global spin flip. If the boundary conditions are symmetric, then ρ_L has an infinite-volume limit (which is the mixture $\frac{1}{2}\rho^+ + \frac{1}{2}\rho^-$).

Proof. Let ρ be any limit of ρ_L along some subsequence of L 's. ρ is a Gibbs state and hence can be expressed uniquely²⁰ as a mixture of the pure Gibbs states: $\rho = \alpha\rho^+ + (1-\alpha)\rho^-$ for some $0 \leq \alpha \leq 1$. But since each ρ_L has all odd correlations vanishing, so does ρ . Therefore, ρ is invariant under a spin flip. On the other hand, since ρ^+ and ρ^- transform into each other under a spin flip, ρ must transform into $\alpha\rho^- + (1-\alpha)\rho^+$. This requires that $\alpha = \frac{1}{2}$ and $\rho = \frac{1}{2}\rho^+ + \frac{1}{2}\rho^-$. By a standard compactness argument, if all subsequence limits are the same ρ , then $\rho_L \rightarrow \rho$ over the entire sequence.

The next theorem is the main rigorous result of this

section. It is our first step in arguing that the SK picture leads to chaotic L dependence. The theorem concerns finite-volume Gibbs distributions whose \mathcal{J} -independent boundary conditions are *flip related*. By this we mean that for each L , there is some subset B_L of the boundary of Λ_L whose flip transforms each boundary condition into the other. An example of such a pair is periodic and antiperiodic; e.g., if the antiperiodicity is only along the j th coordinate axis ($j=1$ or 2 or . . . or d), then B_L consists of one of the two faces of the boundary of Λ_L which are perpendicular to that axis. A second example is any two fixed boundary configurations; here B_L is of course just the set of sites where the two boundary configurations differ. A third example has as the first boundary condition the mixture (with equal weights) of some fixed boundary configuration and its total flip and the second boundary condition the similar mixture for any other fixed boundary condition; the B_L is as in the second example. An example of flip-*unrelated* boundary conditions is periodic and fixed. The theorem requires the common distribution of the J_{ij} 's to be symmetric, i.e., invariant under $J_{ij} \rightarrow -J_{ij}$ and as usual we deal with spin glasses with no external field.

Theorem 3. Assume a symmetric coupling distribution. Consider two \mathcal{J} -independent flip-related boundary conditions and the corresponding ρ_L^1 and ρ_L^2 . If (for almost all \mathcal{J}), ρ_L^1 has an infinite-volume limit, then the same is true for ρ_L^2 and the two limits are the same.

Proof. Consider the correlation function of the spins at the m distinct sites i_1, \dots, i_m as in (5). For each L , call this m -point correlation function X_L^1 for boundary condition 1 and X_L^2 for boundary condition 2. X_L^1 and X_L^2 are functions of \mathcal{J} as is $X = \lim_{L \rightarrow \infty} X_L^1$. We need to show first that $X^2 = \lim_{L \rightarrow \infty} X_L^2$ exists and second that $X^2 = X^1$ (for almost all \mathcal{J}).

Let G denote the (infinite volume) spin flip transformation relating the two boundary conditions; i.e., G flips S_x for each x which belongs to B , the union of all the subsets B_L of the boundary of Λ_L (discussed above), and let \hat{G} denote the corresponding transformation on \mathcal{J} . That is, \hat{G} replaces J_{ij} by $-J_{ij}$ for each i, j with exactly one of the sites in B . Let $\eta = +1$ or -1 according to whether $\{i_1, \dots, i_m\}$ contains an even or odd number of sites from B . Then (for L large enough so that $\{i_1, \dots, i_m\} \subset \Lambda_L$)

$$X_L^2(\mathcal{J}) = \eta X_L^1(\hat{G}\mathcal{J}). \tag{6}$$

Let A denote the set of \mathcal{J} 's for which $X_L^2(\mathcal{J})$ has a limit; by assumption A has probability one. By (6), the set of \mathcal{J} 's for which $X_L^2(\mathcal{J})$ has a limit is $\{\mathcal{J} : \hat{G}\mathcal{J} \in A\}$. But the assumption of symmetry on the coupling distribution implies that this set has the same probability as A ; thus X_L^2 has a limit for almost all \mathcal{J} .

It remains to show that $X(\mathcal{J}) \equiv X^1(\mathcal{J}) - X^2(\mathcal{J}) = 0$ for almost all \mathcal{J} . X is the limit of $X_L \equiv X_L^1 - X_L^2$. Note that X_L^1 and X_L^2 are bounded between -1 and 1 for all L and all \mathcal{J} . We now focus on the conditional expectation $E_r[\cdot]$, defined as the expectation of a quantity after averaging over all of the couplings outside of the cube Λ_r ;

hence $E_r[\cdot]$ is a function of all couplings J_{ij} with both i and j in Λ_r . Because

$$E_r[X_L] = E_r[X_L^1] - E_r[X_L^2], \quad (7)$$

then

$$E_r[X] = \lim_{L \rightarrow \infty} (E_r[X_L^1] - E_r[X_L^2]). \quad (8)$$

Now for a given r , let $L \geq r$ (and large enough so that $\{i_1, \dots, i_m\} \subset \Lambda_L$). Because $E_r[\cdot]$ averages over the boundary bonds of the cube, we claim that $E_r[X_L^2] = E_r[X_L^1]$ due to the spin flip which connects the pair of boundary configurations (and due to the symmetry of the J_{ij} distribution). To see this, do a simpler gauge transformation than the one used to derive (6); namely, just flip each S_x with x in B_L and the corresponding couplings between B_L and Λ_L . Therefore, $E_r[X] = 0$ for every r . But if the random variable X (which is bounded, hence integrable) has a conditional expectation equal to zero for every r , then $X = 0$ (for almost all \mathcal{F}).²² The theorem now follows, because the same argument is true of all correlation functions.

For the remainder of this section we restrict attention to \mathcal{F} -independent symmetric boundary conditions, such as periodic. We argue, first for zero temperature and then for nonzero (low) temperature that within the SK picture it is implausible to have the same infinite-volume limit for all flip-related boundary conditions. The only way to avoid this implausible situation, according to Theorem 3, is for the limit not to exist; i.e., to have chaotic L dependence.

For the rest of this section we require that the distribution of the J_{ij} 's be continuous. This eliminates accidental energy degeneracies and implies that for, say, periodic (or flip-related) boundary conditions on Λ_L , there is (for almost all \mathcal{F}) a unique pair of ground-state configurations related by a global spin flip: $S^L = (S_i^L; i \in \Lambda_L)$ and $-S^L$. S^L will of course depend on the particular boundary condition. At $T=0$, ρ_L is the symmetric (i.e., with equal weights) sum of two δ functions on S^L and $-S^L$. In this situation, $\rho_L \rightarrow \rho$ means simply that ρ is the symmetric sum of δ functions on some infinite space spin configuration $S = (S_i; i \in \mathbb{Z}^d)$ and $-S$ and that for each fixed i , $S_i^L = S_i$ for all large L (how large may depend on i).²³ Any such S must automatically be an infinite-volume ground state (i.e., a configuration such that the flip of *any* finitely many spins raises the energy) and the pure Gibbs states are simply the δ functions on infinite-volume ground states. They of course come in pairs related by a global spin flip.

According to the SK picture, there are *many* pairs of infinite-volume ground states. If, with periodic boundary conditions, ρ_L has an infinite-volume limit (for almost all \mathcal{F}), then it means that a *single* (\mathcal{F} -dependent) pair persists in the limit $L \rightarrow \infty$, and moreover that *same* pair persists for *any* flip-related boundary condition (such as antiperiodic). This would mean that among all the many pairs of ground states, one pair would have an extra stability property guaranteeing it would be the one chosen by *any* \mathcal{F} -independent boundary condition (flip-related to

periodic); other pairs could only be chosen by \mathcal{F} -dependent boundary conditions. This already seems implausible to us.

But let us pursue the matter further. Consider the \mathcal{F} -independent boundary condition which is a symmetric mixture of some fixed boundary configuration with its total flip. Although Theorem 3 does not imply it, we would expect that if periodic boundary conditions have a limit, then so does this other \mathcal{F} -independent (but flip-unrelated to periodic) boundary condition, and furthermore that the limit is the same. If that is so, then it ought to be the case that any \mathcal{F} -independent symmetric boundary conditions would yield the same pair of (infinite-volume) ground states, even though many ground states exist; i.e., all but one of the ground states would be invisible to \mathcal{F} -independent boundary conditions. Such a situation corresponds to neither of the standard pictures, but is reminiscent more of the scaling than the SK picture (and so in Sec. IV we call it the weak scaling picture). We conclude that, at zero temperature, chaotic L dependence is required by any reasonable SK scenario. With chaotic L dependence, different ground states would be visible for \mathcal{F} -independent boundary conditions by choosing \mathcal{F} -dependent subsequences of L 's.

We next consider positive temperatures. If ρ_L with periodic boundary conditions has an infinite-volume limit (for almost all \mathcal{F}), then that limit ρ is a unique mixture of all the pure Gibbs states: either a countable sum,

$$\rho = \sum_{\alpha} W_{\alpha} \rho^{\alpha}, \quad (9)$$

or possibly an analogous integral over continuously many pure states. The latter possibility already seems inconsistent with the conventional SK picture in which most of the weight in such a decomposition comes from a finite number of pure states.¹⁵ In either case, what seems most implausible within the SK picture is that, according to Theorem 3, changing from periodic to antiperiodic (or *any* flip-related) boundary conditions would not only not change the ρ^{α} 's but would also leave the weights W_{α} unchanged. This is implausible: states which at low T contribute to the sum in Eq. (9) must in some sense have free energy differences of order one (or they would have vanishing Boltzmann weights), so that introduction of at least one relative domain wall (occurring in the switch from periodic to antiperiodic boundary conditions) must necessitate significant changes in relative weights (if the set of ρ^{α} 's is not replaced altogether). We therefore conclude that it is unlikely that the limiting state is a mixture of many states; surely, it should be a mixture of only two states, related by a global spin flip. Finally, if the limit does indeed exist, i.e., $\rho_L \rightarrow \rho$, for periodic boundary conditions, then just as for $T=0$, we would expect that any \mathcal{F} -independent (and symmetric) boundary condition should also have the same ρ as a limit. But such insensitivity to boundary conditions is contrary to the nature of the SK picture. Our conclusion is that any reasonable SK picture requires chaotic L dependence; its nature within various versions of the SK scenario will be discussed in Sec. V.

III. EXAMPLES OF CHAOTIC SIZE DEPENDENCE

In this section we demonstrate by several examples that chaotic size dependence is a natural occurrence in many disordered systems. The first and most important example is within the infinite-ranged SK model itself.

The SK model,⁴ for size N , consists of Ising spins S_i , $i=1, \dots, N$, with Hamiltonian

$$\mathcal{H} = -N^{-1/2} \sum_{i>j=1}^N J_{ij} S_i S_j, \quad (10)$$

where the couplings J_{ij} are again chosen with quenched, independent randomness with some common distribution, which may be taken to be Gaussian [Eq. (4)]. (We use the same notation for J_{ij} and \mathcal{J} even though the indices differ from the short-ranged case.) Let $\rho_N = \rho_N^{\mathcal{J}}$ denote the Gibbs distribution, at some fixed T , for Eq. (10) (there are no boundary conditions here) and let ρ'_N denote a Gibbs distribution for duplicate variables S'_i (with the same \mathcal{J}). The joint probability measure $\bar{\rho}_N$ for the pair (S, S') of spin configurations is the product of ρ_N and ρ'_N ; we denote by $\langle \cdot \rangle_N$ its thermal average. The size- N order parameter distribution for fixed couplings, $P_N^{\mathcal{J}}(q)$, is simply the probability distribution of the overlap sum,

$$Q \equiv (1/N) \sum_{i=1}^N S_i S'_i. \quad (11)$$

It is a \mathcal{J} -dependent sum of δ -functions on $[-1, 1]$ whose Laplace transform is

$$Y_N^{\mathcal{J}}(t) \equiv \int_{-1}^1 e^{tq} P_N^{\mathcal{J}}(q) dq = \langle e^{tQ} \rangle_N. \quad (12)$$

The average of $P_N^{\mathcal{J}}(q)$ over \mathcal{J} , $[P_N^{\mathcal{J}}(q)]_{\text{av}}$, is the quantity studied numerically in Ref. 12. According to the Parisi solution¹⁵ $P_N^{\mathcal{J}}(q)$ should be non-self-averaging,²⁴ i.e., should have nontrivial dependence on \mathcal{J} , even as $N \rightarrow \infty$. In particular, a quantity like $Y_N^{\mathcal{J}}(t)$,²⁵ regarded as a function of \mathcal{J} , should have nontrivial fluctuations:

$$\text{Var}(Y_N^{\mathcal{J}}(t)) \equiv [Y_N^{\mathcal{J}}(t)^2]_{\text{av}} - ([Y_N^{\mathcal{J}}(t)]_{\text{av}})^2 \quad (13)$$

should not tend to zero as $N \rightarrow \infty$. The next theorem shows that such non-self-averaging requires chaotic N dependence of $P_N^{\mathcal{J}}(q)$. For a given \mathcal{J} , we say that $P_N^{\mathcal{J}}(q)$ has a limit as $N \rightarrow \infty$ if $Y^{\mathcal{J}}(t) \equiv \lim_{N \rightarrow \infty} Y_N^{\mathcal{J}}(t)$ exists for each real t ; there is then a unique probability measure $P_{\mathcal{J}}$ on $[-1, 1]$ whose Laplace transform equals $Y_{\mathcal{J}}$.

Theorem 4. If $P_N^{\mathcal{J}}(q)$ has a limit $P^{\mathcal{J}}$ (for almost all \mathcal{J}),²⁶ then there is self-averaging in the sense that $P^{\mathcal{J}}$ is equal to a fixed \mathcal{J} -independent P (for almost all \mathcal{J}) and also for each real t ,

$$\text{Var}(Y_N^{\mathcal{J}}(t)) \rightarrow 0 \quad \text{as } N \rightarrow \infty. \quad (14)$$

Proof. Suppose \mathcal{J} and \mathcal{J}' differ for only finitely many \mathcal{J}_{ij} 's. Then a comparison of the size- N Gibbs distributions shows that because of the $N^{-1/2}$ factor in the SK Hamiltonian (10),

$$Y_N^{\mathcal{J}'}(t) / Y_N^{\mathcal{J}}(t) = e^{O(N^{-1/2})}. \quad (15)$$

Thus $Y^{\mathcal{J}'}(t) = Y^{\mathcal{J}}(t)$. Because this is true for any such re-

lated \mathcal{J} and \mathcal{J}' , it follows from the Kolmogorov zero-one law that for each fixed t , $Y^{\mathcal{J}}(t)$ is a constant (for almost all \mathcal{J}). This implies that $P^{\mathcal{J}}$ is independent of \mathcal{J} (for almost all \mathcal{J}). Since for fixed t , $Y_N^{\mathcal{J}}(t)$ converges to a constant (for almost all \mathcal{J}), and since the $|Y_N^{\mathcal{J}}(t)|$ are bounded functions of \mathcal{J} (by $e^{|t|}$) uniformly in N , it follows that $\text{Var}(Y_N^{\mathcal{J}}(t))$ converges to zero (the variance of a constant).

We proceed with brief discussions of four examples where chaotic size dependence occurs in finite-ranged disordered systems. The first is our EA d -dimensional spin glass at zero temperature, but now with plus boundary conditions or any other fixed \mathcal{J} -independent boundary configuration. We assume a symmetric and continuous coupling distribution. Now since there is a fixed boundary configuration, ρ_L is a δ function on a single ground-state configuration (rather than on a pair, as occurs with symmetric boundary conditions). Hence if ρ_L has a limit, it is also supported on a single (infinite volume) ground state. Now consider the boundary conditions obtained from a global spin flip of the previous boundary conditions. On the one hand, these would clearly yield the global spin flip of the previous limit; on the other hand, by Theorem 3 the two limits must be the same. This contradiction was a consequence of the assumption that ρ_L has a limit for almost all \mathcal{J} ; we conclude that there must be chaotic L dependence. Within the scaling picture this chaotic dependence simply corresponds to the spin at the origin never settling down to a fixed sign as $L \rightarrow \infty$ — the fixed boundary condition sometimes prefers one of the two (infinite volume) ground states and sometimes the other (its global spin flip). This phenomenon should persist within the scaling picture also for $T > 0$ as the fixed boundary condition sometimes prefers the pure state ρ^+ and sometimes ρ^- . Within the SK picture, the system may alternate among many ground states. Here things are even more chaotic, as (some) pair and higher even-spin correlations should also fail to have a limit as $L \rightarrow \infty$. Once again, we expect the phenomenon to persist at positive temperature; most likely, chaotic L dependence will occur at any temperature in which global spin flip symmetry is broken (i.e., the Edwards-Anderson order parameter q_{EA} is nonzero).

The next example is an artificial construction designed to illustrate more explicitly how nonexistence of a limit may occur in a spin glass. (We note, however, that the mechanism involved in this example may be, and in the last two examples certainly is, related more to nonexistence of a limit in the scaling picture when nonsymmetric boundary conditions are employed, rather than in an SK picture with periodic boundary conditions.) Consider a two-dimensional nearest-neighbor Ising model on a square lattice, with all couplings equal to $+J$ except those oriented vertically and connecting the $y=0$ to the $y=1$ line: these are chosen independently to be $\pm J$, each with probability $\frac{1}{2}$. Now consider at $T=0$ the sequence of squares Λ_L , all with free boundary conditions. For each square, one of two states will be obtained: the first is the mixed state composed of all spins up or all down, with equal probability; the second is the mixed state com-

posed of all spins up in the top half and all down in the bottom, or *its* global spin flip, again with equal probability. Which state is actually chosen depends on the sign of the sum of the randomly chosen couplings; if the sum is positive, the first state will be selected, and if negative, the second. Now, as $L \rightarrow \infty$ *independently* of the couplings, this sum will execute a one-dimensional random walk, with its sign changing infinitely often between plus and minus. In this case, a limit will not exist.

In this example, two different limiting Gibbs distributions *can* be found if some subset of the L 's are chosen *dependently* on the couplings. That is, one could choose only those L 's such that the sum of the randomly chosen couplings is positive; in that case one would select out the first Gibbs distribution in the infinite-volume limit. Similarly, by choosing L 's such that the sum is always negative, one generates the second Gibbs state. This illustrates an important property of all such cases in which nonexistence of a limit occurs, including the spin glass itself: any nonconvergent sequence of boundary conditions always contains convergent (but \mathcal{J} -dependent) subsequences. This follows from standard compactness arguments.

However, in contrast to the spin glass (within the SK picture), not *all* sequences of coupling-independent boundary conditions have the property of nonexistence of a limit; in fact, many do have a limit. For example, periodic boundary conditions in the y direction will always select out the first Gibbs state.

The next example⁸ is the three-dimensional random field Ising model with, say, a Gaussian distribution of fields with zero mean. At sufficiently low temperature, a sequence of either free or periodic boundary conditions with L chosen independently of the fields will not yield a limiting Gibbs distribution, owing to the oscillation in sign of the sum of the random fields as the volumes grow. (Again, one *can* obtain a limit by choosing L dependently on the fields.) Here, however, a sequence of deterministically chosen *fixed* boundary conditions, such as all spins up at the boundary, does yield a limit on any sequence of volumes, unlike in the spin-glass case.²⁷

The last example is a two-dimensional ferromagnet in zero external field. If for each L the boundary spins are chosen randomly and independently (say, by flipping a fair coin at each site on the boundary), then there will be no limit owing to the oscillation in sign of the sum of the boundary spins. This phenomenon is rather clear at $T=0$ and has been discussed previously;²⁸ it should persist also at nonzero temperature and higher dimension.

Now that our main result—the close connection between existence or nonexistence of a limit using periodic boundary conditions with the question of multiple Gibbs states—has been discussed in some detail, we turn to a closer examination of each of the two opposing viewpoints of short-ranged spin glasses. We first discuss the scaling picture.

IV. SCALING PICTURE

Until now we have not needed to categorize the relationships between pure states which may arise in short-ranged spin glasses. A lucid discussion may be found in

Ref. 8, whose definitions we adopt here. We focus on two possible relationships among pure states which are not trivially related (i.e., not related by a global spin flip): *incongruent* and *regionally congruent*. Incongruent states are unrelated by any simple symmetry. At $T=0$, two incongruent ground states possess a nonvanishing density of relative domain walls. (A specific bond belongs to a relative domain wall between two spin configurations if it is satisfied in one configuration and not the other.) Regionally congruent ground states, on the other hand, possess a vanishing density of domain walls. We refer the reader to Ref. 8 for a more complete discussion. When we do not need to distinguish between incongruent or regionally congruent states, we will use the term “noncongruent,” which includes both.

Because we consider, in this section, sequences only of \mathcal{J} -independent symmetric boundary conditions, we focus on incongruent states; we do not believe that regionally congruent states, which in all known cases arise from boundary conditions carefully tailored to the couplings, present an issue here. We will assume throughout this section that a limit as $L \rightarrow \infty$ with periodic boundary conditions exists (for almost all \mathcal{J}), which we argued in Sec. II implies the correctness of the scaling scenario. Our aim in this section is to examine more closely the consequences of the existence of this limit, and show that a self-consistent picture emerges. We do this through an examination of the likely volume dependence of energy differences between incongruent ground states; our conclusions will also be relevant for the discussion of numerical simulations in the next section.

Fisher and Huse (FH) have examined^{8,9} the conditions under which incongruent states will and will not occur; their argument amounts to comparing bulk free-energy fluctuations arising from incongruence to those due to different boundary conditions. We paraphrase here their main argument (restricted to the case $T=0$), and refer the reader to the original papers for details.

Consider the Ising spin-glass model with Hamiltonian (3) and a symmetric coupling distribution such as (4) in Λ_L , and ask what ground-state energy difference would result from two separate boundary conditions. Numerical results^{5,6} and the droplet picture⁷ suggest that the root mean square difference will be no larger than the square root of the boundary area, or $\sqrt{L^{d-1}}$. This is the assertion²⁹ that the scaling exponent $\theta \leq (d-1)/2$. (Bray and Moore use the symbol γ for the same exponent.⁶)

Suppose for a moment that incongruent ground states do exist, and consider two such infinite-volume states for the same \mathcal{J} . Now consider the energy for each contained within the volume Λ_L . A central question concerns typical energy differences within this volume; if they are of order unity, then incongruent states should easily arise from different boundary configurations. However, FH argue that *their* typical energy difference is bounded from below by $\frac{\sqrt{L^d}}{\sqrt{L^{d-1}}}$, which would presumably violate the bound ($\sqrt{L^{d-1}}$) on maximal energy differences which can be gotten by switching from periodic to antiperiodic boundary conditions.⁹ The implication is then that any two \mathcal{J} -independent sequences of boundary conditions will not generate incongruent states.

Nevertheless, this does not completely rule out incongruent states, as FH recognized.⁹ It could be that for a fixed realization \mathcal{J} , special boundary conditions *depending* on \mathcal{J} might be found, with an energy difference of order $L^{\bar{\theta}}$. (See Ref. 9 for a more precise definition of $\bar{\theta}$). In general, $\theta \leq \bar{\theta} \leq d-1$; FH assumed that $\theta = \bar{\theta}$, but the issue is unresolved. In particular, if $\bar{\theta} \geq d/2$, then incongruent ground states can exist even if they have free energy differences scaling with the square root of the volume. In this case, however, boundary conditions chosen *independently* of the couplings cannot generate incongruent states; they can only arise from special choices of sequences of boundary conditions dependent on the couplings.

Summarizing, there are three main possibilities: (1) Low-lying (in energy) incongruent states have bulk energy differences of order one, independent of the volume. In this case they would be generated by any two different sequences (say, periodic and antiperiodic) of boundary conditions. (2) Low-lying incongruent states cannot have energy differences less than order square root of the volume, and moreover the exponent $\bar{\theta} \leq (d-1)/2$. In this case, incongruent states do not exist. (3) Low-lying incongruent states have energy differences of order square root of the volume, and the energy difference between two \mathcal{J} -independent boundary conditions is bounded by the square root of the enclosing area, but the *maximal* energy difference can be greater. Special \mathcal{J} -dependent choices of boundary conditions may then generate incongruent states, but in general two boundary conditions, chosen independently of the couplings, will not.

We now argue that the existence of incongruent states with $O(1)$ bulk energy differences is incompatible with existence of a limit for \mathcal{J} -independent (e.g., periodic) boundary conditions. If there are many such states, then which is the actual bulk ground state should depend on L . But this contradicts the requirement that the limit exists. We conclude that if periodic boundary conditions possess a limit as $L \rightarrow \infty$ (for almost all \mathcal{J}), then the typical energy difference between incongruent states, both within Λ_L , should scale as $\sqrt{L^d}$. In principle, one could argue that the difference has only been shown to scale as L^x , with $x > 0$ (or diverge even more slowly), but there is no apparent reason why x should be anything between 0 and $d/2$, and so we do not pursue this further.

We have provided heuristic reasons why one part of the FH argument follows from existence of a limit; the other part, i.e., the inequality $\theta \leq (d-1)/2$, has been rigorously proved by Aizenman and Fisher.³⁰ Their result, a version of which is given in the following theorem, can be proved by applying techniques similar to those used by Aizenman and Wehr in studying the random field Ising model.³¹

Theorem 5. Consider the Ising spin-glass Hamiltonian (3) with a symmetric coupling distribution at some fixed temperature (positive or zero) in zero external field. Given two flip-related boundary conditions on $\partial\Lambda_L$, the surface of Λ_L ,

$$\text{Var}(F_1 - F_2) \leq 4 \text{Var}(J_{ij}) |\partial\Lambda_L|, \quad (16)$$

where F_1 and F_2 denote the respective free energies with boundary conditions 1 and 2, and $\text{Var}(X)$ is the variance of X with respect to averaging over the coupling distribution.

An immediate consequence of Theorem 5 is that, for a typical realization \mathcal{J} in a volume Λ_L , the free energy difference between two flip-related boundary conditions, chosen independently of the couplings, is bounded by a number which scales as $\sqrt{L^{d-1}}$. This suggests that if two incongruent states in Λ_L possess typical free energy differences of order $\sqrt{L^d}$, they will not both be “seen” in Λ_L by choosing two flip-related boundary conditions, such as periodic and antiperiodic, so long as L is chosen independently of the couplings. This is a kind of strengthening of the remarks made following Theorem 3, which dealt only with infinite-volume limits rather than estimates for large finite L .

Further, if the exponents θ and $\bar{\theta}$ are equal, then Theorem 5 suggests that no incongruent states exist at all. If $\bar{\theta} > \theta$, on the other hand, then we are also left with the possibility that multiple Gibbs states exist, but all coupling-independent sequences of boundary conditions will always choose the same one. This might be called the “weak” scaling picture. The “exotic” states should probably be regarded as unphysical. One reason for supposing this³² is the finding³³ that similar exotic states actually occur in long-ranged spin-glass models *at all temperatures*, coupled with the knowledge that at least at high temperature the single (paramagnetic) state seems unaffected.³⁴

V. SK PICTURE AND NUMERICAL SIMULATIONS

Until now we have argued that a naive version of the SK picture for short-ranged models (i.e., a sequence of periodic boundary conditions having an infinite-volume limit which consists of a mixture of many pure states) cannot hold, and must be replaced by a picture in which such a limit does not exist. In this section we assume that multiple incongruent pure states do exist, and examine possible SK-like pictures consistent with the resulting chaotic size dependence. We present a heuristic discussion in which we propose two such plausible SK-like pictures; one is similar to the zero temperature picture of Sec. II, while the other is considerably different. In particular, we investigate what it means for multiple states to coexist under a *single* choice of boundary conditions. This is of particular interest because almost all numerical simulations which search for multiple states do so using a single set of boundary conditions, usually periodic.^{2,11,12,35}

Throughout the following discussion, we will assume that bulk free-energy differences between noncongruent pure states are of order one,³⁶ otherwise, we would be back to some version of the scaling picture, as discussed in the last section. Within this assumption, however, there are still various possibilities; we consider here the two most obvious ones. The first is that two noncongruent pure states (of infinite extent) may have a bulk free-energy difference of order one in a fixed volume, but may in general not be compatible with the same set of boundary conditions. This would be reminiscent of the

situation at zero temperature, in which only one ground state and its global flip exists on any finite volume (for continuous couplings). The second possibility is that many pure states not only have free energy differences of order one in bulk, but are also compatible with the same set of boundary conditions, such as periodic. Then in any finite volume several such states will contribute to the Boltzmann sum, as in the infinite-ranged model.

In the first case, a single set of boundary conditions will be insufficient for the observation of incongruence. It is presumably the second possibility which numerical simulations are searching for.

As already mentioned, such simulations almost invariably use periodic boundary conditions on one or a few cubes chosen independently of the couplings. In recent papers which search for incongruence, two measures are employed; the simulations by Reger *et al.*¹² measure the usual spin overlap function $P(q)$ on several four-dimensional hypercubes, while the three-dimensional simulations of Caracciolo *et al.*¹¹ measure both $P(q)$ and a "link-link" overlap function P_e (defined in their paper, but which essentially measured the distribution of the spatial average of $\langle S_i S_j \rangle \langle S'_i S'_j \rangle$). Of the two measures, only P_e is sensitive to the difference between incongruence and regional congruence.

While the results of both papers are intriguing, and seem consistent with an SK-like picture,³⁷ neither can be regarded as conclusive for several reasons. Some are obvious: because of small lattice sizes, finite volume effects may be substantial. Simulations are carried out at moderately high temperatures, where even in the scaling picture noncongruence will arise due to thermal excitations. (On the other hand, we remark that when dealing with a single boundary condition, the amount of incongruence can be proved to be bounded above by $k_B T$ regardless of the number of pure states.³⁸) The effects of this thermally induced incongruence must somehow be disentangled from the sought-after "quenched" incongruence; separating these effects may be difficult for some lattices. Moreover, in the Caracciolo *et al.* simulations, a discrete distribution for the couplings is used, which can lead to accidental degeneracies whose effects on small lattices may be pronounced. A more detailed critique of both simulations, particularly those of Caracciolo *et al.*, is given in Ref. 37.

We emphasize that these objections can in principle be overcome in obvious ways (although it may be difficult to do so in practice). More serious is a problem which has been pointed out by Huse and Fisher,^{8,37} who provided an example (the two-dimensional Ising ferromagnet on a square lattice with antiperiodic boundary conditions in both directions) in which there are only two pure states, and yet $P(q)$ (as studied numerically) remains nontrivial even in the infinite-volume limit. [We agree, however, with Reger *et al.* that $P(q)$ still contains interesting information. The number of pure states refers to knowledge about all sets of local correlations, but loses information about the global nature of the state generated in any finite volume. This last piece of information may be important both numerically and experimentally, and is conveyed by the $P(q)$ function.] Moreover, even if

the scaling picture is wrong, $P(q)$ can still be a pair of δ functions if the first of our two alternative SK pictures holds. In this case, even though there are many states, no more than two (related by a trivial spin flip) will coexist in a typical Λ_L . We therefore propose a test to surmount these difficulties.

Consider two cube sizes $L_1 < L_2$. In going from L_1 to L_2 , either: (a) a wholly or partially new set of pure states is picked out, or (b) the same set remains but with different weights, or (c) some combination of the above.³⁹ One can in principle test for such an occurrence: consider some subvolume of the smaller cube, well away from the boundary. Pick out some set of two- and maybe four-point correlation functions, and measure their values. If the above scenario does occur, then one should see a dramatic change in the correlation functions in going from cube 1 to cube 2. On the other hand, if all of the incongruence seen is simply thermally induced, only minor changes will be seen, because cube 2 generates (almost) the same state in bulk as cube 1. Therefore, after many such trials, and using several different coupling realizations, it should become clear which kind of incongruence is actually being seen. Such a test directly looks for the chaotic L dependence previously discussed. We caution that we have no information about how frequently changes in state should occur; however, if (as in the standard SK picture) there really is an infinite set of incongruent pure states, it seems unreasonable that, say, doubling the cube size would pick out the same states with the same weights.

A test such as the one discussed above should be used in conjunction with another employing two sets of boundary conditions. In such a test, one might focus on a (not too small) Λ_L , and surround it with an appreciably larger cube $\Lambda_{L'}$. Select fixed boundary conditions on the surface $\partial\Lambda_{L'}$ for one trial, and an independent set of boundary conditions for a second trial. For increasing sequences of the size L' , study the evolution of the bond overlap function P_e between configurations in Λ_L corresponding to the different boundary conditions. Repeat this procedure at the lowest feasible temperature for as many different sets of boundary conditions as is possible.

In both of the tests suggested above, measurements at the lowest possible temperature is suggested, in order to minimize the effects of thermally induced incongruence. In practice, these tests, particularly the one employing two sets of boundary conditions, are difficult to execute, due to long thermalization times; on the other hand, such tests help to remove possible ambiguities of the kind discussed in this section. We also suggest avoiding discrete distributions, because, for lattice sizes likely to be studied numerically, a fraction of domain walls between two configurations at low temperature will be present due simply to local degeneracies. Finally, we point out that, if all of the above conditions are met, and even if a simple scaling picture holds, there will still be some incongruence seen as the lattice size increases, due to relative domain walls. However, the fraction of bonds these domain walls occupy would be subextensive, and as L increases this fraction would fall to zero as a power of L .

To summarize, we propose a numerical test to look

directly for chaotic size dependence, which differentiates between the scaling and SK pictures for short-ranged models. [Another chaotic dependence, on changing temperature for fixed volume, may also occur, but probably does not differentiate between the two pictures. It has been argued^{40,16} that chaotic temperature dependence follows from the bound $\theta \leq (d-1)/2$; if so, it holds for short-ranged models, regardless of whether the scaling or SK picture is valid.] We have proposed two possible ways in which an SK picture may hold for short-ranged models. If the second of these holds, our test goes beyond that of looking for a nontrivial $P(q)$. If the first holds, $P(q)$ will be trivial but chaotic size-dependence will remain. If the scaling picture is right, a chaotic size

dependence cannot occur. In all cases, our test is more sensitive than those which look for nontrivial $P(q)$, which does not carry unambiguous information about the number of pure states.

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¹⁸Although we believe that Theorem 1 should be valid at zero temperature, the proof given is not applicable to that case.

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²⁰H.-O. Georgii, *Gibbs Measures and Phase Transitions* (W. de Gruyter, Berlin, 1988).

²¹If there is a unique Gibbs state (for almost all \mathcal{J}), then of course there is no chaotic L dependence for any choice of boundary conditions. This is the case at high temperature, and according to the scaling picture (see Ref. 16) would also be the case for any nonzero external field.

²²This follows by a standard application of the martingale convergence theorem; see, e.g., K. L. Chung, *A Course in Probability Theory*, 2nd edition (Academic, New York, 1974).

²³We have arranged notation so that at the origin, $S_0 = +1$ and $S_0^L = +1$ for all L .

²⁴Non-self-averaging has been proved rigorously in the SK model for the EA order parameter in the presence of a random symmetry-breaking field; see L. A. Pastur and M. V. Shcherbina, *J. Stat. Phys.* **62**, 1 (1991).

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²⁶The proof of this theorem also shows, as in Theorem 1, that either $P_{\mathcal{N}}^{\mathcal{J}}(q)$ has a limit for almost all \mathcal{J} or almost none. We also remark that the hypothesis can be weakened to convergence of $Y_{\mathcal{N}}^{\mathcal{J}}(t)$ to some limit $Y^{\mathcal{J}}(t)$ in probability (rather than for almost all \mathcal{J}); i.e., $\bar{\rho}_{\mathcal{N}}(\{(S, S') : |Y_{\mathcal{N}}^{\mathcal{J}}(t) - Y^{\mathcal{J}}(t)| \geq \epsilon\}) \rightarrow 0$ for each ϵ . Further, this need only be valid for a countable (dense) set of t 's.

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- ³⁸The result is that if J_{ij} has a probability density function bounded by C , then $[1 - \langle S_i S_j \rangle^2]_{\text{av}} \leq 2Ck_B T$; C. M. Newman and D. L. Stein, unpublished.
- ³⁹In the first SK scenario we proposed, only a single state (modulo a spin flip), will contribute to the Boltzmann sum in each cube, but the state will eventually change as L increases. This situation will presumably occur in the second SK scenario only at zero temperature. In either case our suggested test will still work.
- ⁴⁰A. J. Bray and M. A. Moore, *Phys. Rev. Lett.* **58**, 57 (1987).