Non-Mean-Field Behavior of Realistic Spin Glasses

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We provide rigorous proofs which show that the main features of the Parisi solution of the Sherrington-Kirkpatrick spin glass, as applied to more realistic spin glass models, are not valid in any dimension and at any temperature.

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The theoretical perspective provided by the Parisi solution [1] of the infinite-ranged Sherrington-Kirkpatrick (SK) model [2] has dominated the spin glass literature over the past decade and a half. This is partly because it represents the only example of a reasonably complete thermodynamic solution to an interesting and nontrivial spin glass model, and partly because of the novel, and in some respects, spectacular, nature of the symmetry breaking displayed in the low-temperature phase. Its main qualitative features-the presence of (countably) many pure states, the non-self-averaging of their overlap distribution function, and the ultrametric organization of their overlaps, among others-have greatly influenced thinking about disordered and complex systems in general [3,4]. A common working hypothesis is that the Parisi solution provides a theory of general spin glass models [3-5]. In particular, many authors have directly applied its features to the study of both short-ranged models and laboratory spin glasses [6-9]. Support for this "SK picture"-that the main qualitative features of Parisi's solution survive in non-infinite-ranged models-comes from both analytical [10] and numerical [11,12] work.

In this Letter, however, we prove that short-ranged models such as the nearest-neighbor Edwards-Anderson (EA) model [13] have natural thermodynamic states whose overlap distribution functions are self-averaged (i.e., do not depend on the realization J of the couplings). Thus the standard SK picture is not valid. Furthermore, most of our arguments rely on little more than the homogeneity properties of the disorder, and thus are applicable to more realistic spin glass models such as models with long-ranged couplings or diluted RKKY interactions [14].

We do not attempt to resolve in this paper the closely related issue of whether short-ranged spin glass models have many pure thermodynamic states at sufficiently high dimension and low temperature, or only a single pair. The latter conjecture arises from a droplet model [15] based on a scaling *ansatz* [15–17]. Rather, we assert that *if* there are many pure states, their structure and that of their overlaps cannot be that of the SK picture [18].

The SK picture.—The Parisi solution, as applied to the EA model at fixed temperature T, suggests that there exist two related quantities which are non-self-averaging (i.e., depend on J): (i) a state $\rho_J(\sigma)$, which is a Gibbs probability measure (at temperature T) on the microscopic spin configurations σ on all of Z^d , and (ii) a Parisi order parameter distribution $P_J(q)$, which is a probability measure on the interval [-1, 1] of possible overlap values. These two are related as follows: If one chooses σ and σ' from the product distribution $\rho_J(\sigma)\rho_J(\sigma')$, then the overlap

$$Q = \lim_{L \to \infty} |\Lambda_L|^{-1} \sum_{x \in \Lambda_L} \sigma_x \sigma'_x \tag{1}$$

has P_J as its probability distribution. Here $|\Lambda_L|$ is the volume of a cube Λ_L of side length L centered at the origin in d dimensions.

In this picture the decomposition of ρ_J into pure states is *countable* (i.e., a sum rather than an integral):

$$\rho_J(\sigma) = \sum_{\alpha} W_J^{\alpha} \rho_J^{\alpha}(\sigma) \,. \tag{2}$$

If σ is drawn from ρ_J^{α} and σ' from ρ_J^{β} , then the expression in Eq. (1) equals its thermal mean,

$$q_J^{\alpha\beta} = \lim_{L \to \infty} |\Lambda_L|^{-1} \sum_{x \in \Lambda_L} \langle \sigma_x \rangle_\alpha \langle \sigma_x \rangle_\beta \,. \tag{3}$$

Thus P_J is given by

$$P_J(q) = \sum_{\alpha,\beta} W_J^{\alpha} W_J^{\beta} \delta(q - q_J^{\alpha\beta}).$$
(4)

Here, the W_J^{α} 's and $q_J^{\alpha\beta}$'s are non-self-averaging quantities, except for $\alpha = \beta$ or its global flip, where $q_J^{\alpha\beta} = \pm q_{\rm EA}$ (we assume throughout that there is no external field, although that plays no essential role). The average P(q) of $P_J(q)$ over the disorder distribution ν of the couplings is a mixture of two delta-function components at $\pm q_{\rm EA}$ and a continuous part between them.

The countability of the decomposition of Eq. (2) is also employed to obtain the often-used result (see, for example, Refs. [3,6,19]) that the free energies of the lowest-lying states are independent random variables with an exponential distribution.

Both ρ_I and P_I are infinite-volume quantities and so must be obtained by some kind of thermodynamic limit. Naively, one might simply fix J and attempt to take a sequence of increasing volumes with, say, periodic boundary conditions. However, we argued in a previous paper [20] that the existence of multiple pure states is inconsistent with the existence of such a limit for *fixed J*. Instead, there would be chaotic size dependence, so that infinite-volume limits can be achieved only through coupling-dependent boundary conditions. We will see below that, nonetheless, ρ_I and P_I can be obtained by natural limit procedures which are coupling independent and which imply translation covariance for ρ_{I} [21,22] and translation invariance for P_{I} . We ask whether this is consistent with the SK picture, which requires the following properties of P_{I} and its average P: (1) $P_I(q)$ is non-self-averaging. (2) $P_I(q)$ is a sum of (infinitely many) delta functions. (3) P(q) has a continuous component (for all q between the delta functions at $\pm q_{\rm EA}$).

The answer is no; we will see that *translation invariance rules out non-self-averaging*. This in turn makes the absence of a continuous component in P_J inconsistent with its presence in P. We conclude that property (1) is absent, and at most one of the remaining two properties can be valid for realistic spin glass models. We will consider below the implications of this result for other important features of this picture, such as ultrametricity.

Construction of ρ_J and P_J .—We first describe a limit procedure to obtain P_J which does not involve the prior construction of ρ_J . Begin with the finite-volume Gibbs distribution $\rho_{J^{(L)}}^{(L)}$ on the spin configuration $\sigma^{(L)}$ in the cube Λ_L with periodic boundary conditions. Here $J^{(L)}$ denotes the couplings restricted to Λ_L . Let $Q^{(L)}$ denote the overlap of $\sigma^{(L)}$ and a duplicate $\sigma^{l(L)}$:

$$Q^{(L)} = |\Lambda_L|^{-1} \sum_{x \in \Lambda_L} \sigma_x^{(L)} \sigma_x^{\prime(L)}.$$
 (5)

The distribution $P_{J^{(L)}}^{(L)}$ for $Q^{(L)}$ is the finite-volume Parisi overlap distribution function, whose average was studied numerically in Refs. [11,12]. It was proved in Ref. [20] that in the SK model, non-self-averaging requires $P_{J^{(L)}}^{(L)}$ to have chaotic *L* dependence as $L \rightarrow \infty$ for fixed *J*; a similar result was suggested, though not proved, for short-ranged spin glasses with many pure states. Because of this, we do not take a limit of $P_{J^{(L)}}^{(L)}$ directly but rather of the *joint distribution* $\tilde{\mu}_L$ of $J^{(L)}$ and $Q^{(L)}$. That is, by a compactness argument (which may require the use of a subsequence of *L*'s) one has a limiting $\tilde{\mu}$, which is a probability measure on joint configurations (J, q) (*q* being a realization of *Q*) such that for any (nice) function *f* of *finitely* many couplings and of *q*, the average $\langle f \rangle$ for $\tilde{\mu}$ is the limit of the averages for $\tilde{\mu}_L$. This gives us existence of a $\tilde{\mu}$, which is a joint distribution on the infinite-volume realizations of J and q. Its marginal distribution for J is the original disorder distribution ν , while its conditional distribution for q given J is what we denote P_J . Because of the periodic boundary conditions, the marginal distribution (under $\tilde{\mu}_L$) of J_1, \ldots, J_m, q is the same (for large L) as of J_1^a, \ldots, J_m^a, q (where a is any lattice translation and J^a is the translated J) and thus one has translation invariance of the limit measure $\tilde{\mu}$. Translation invariance here means that for any a, the shifted variables J^a together with Q have the same joint distribution as do the original J together with Q; because ν is in any case translation invariant, this implies that $P_J = P_{J^a}$. In other words, the overlaps do not care about the choice of origin.

The second and more fundamental procedure for obtaining P_I is first to construct ρ_I and then obtain P_I as the distribution of the Q given by Eq. (1). The construction of ρ_I is as follows [21,22]. Let μ_L be the joint distribution for $J^{(L)}$ and $\sigma^{(L)}$ on the periodic cube Λ_L . Then by compactness arguments, some subsequence μ_L converges to a limiting joint distribution $\mu(J, \sigma)$. The resulting conditional distribution of σ given J is what we denote $\rho_I(\sigma)$. μ will be translation invariant (and ρ_{T} will be translation covariant) because of the translation invariance (on the torus) of μ_L . Translation invariance means that the distribution μ for (J, σ) is the same as for (J^a, σ^a) for any lattice vector a. In terms of ρ_J , this means that $\rho_{J^a}(\sigma) = \rho_J(\sigma^{-a})$, so that, e.g., $\langle \sigma_x \rangle_{I^a} = \langle \sigma_{x-a} \rangle_I$; thus we say that ρ_I is translation covariant rather than invariant. Translation covariance of ρ_{I} immediately implies, via Eq. (1), translation invariance of P_J .

Before pursuing the rigorous implications of translation invariance, we discuss (on a nonrigorous level) several questions related to these constructions. Could different subsequences of cubes yield different limits? We believe the answer is no, although we have no complete proof, because our procedure of considering joint distributions (for J and q or for J and σ) should avoid the kind of chaotic size dependence discussed in Ref. [20]. Could different deterministic boundary conditions yield different limits? Certain classes of boundary conditions must yield the same limit (see Ref. [20]), but in general we cannot rigorously eliminate this possibility. However, we see no mechanism for any such limit to violate the very weak property of translation invariance for P_{I} . Could the P_{I} 's arising from our two constructions (one using ρ_{I} and one not) be different? Yes; in fact, they apparently are different in some models [23]. Either way, since both P_{I} 's are translation invariant, neither one can be nonself-averaging, as we now show rigorously.

Self-averaging of $P_J(q)$.—To prove that translation invariance of $P_J(q)$ implies that it is self-averaging, take a (nice) function f(q) (like q^k) and consider the function of J, $\hat{f}(J) \equiv \int f(q)P_J(q) dq$. By translation invariance,

 $\hat{f}(J) = \hat{f}(J^a)$, but by the *translation ergodicity* [24] of ν , any translation-invariant (measurable) function $\hat{f}(J)$ is equal to its J average, $\int \hat{f}(J)\nu(J)dJ$. Since this is true for all f's, it follows that P_I itself equals its J average.

We remark that this proof is valid for any model involving disorder whose underlying distribution is (like ν) translation invariant and translation ergodic [25]. For example, any analog of the Parisi order parameter distribution for spin glass models with site-diluted RKKY interactions will also be self-averaging (if it is translation invariant).

Because P_I is self-averaging, we are forced to the dichotomy that, for any temperature in any dimension, either $P (= P_I)$ is a sum of one or more δ functions or else P has a continuous component. When there is a unique infinite-volume Gibbs state (e.g., in the paramagnetic phase) then of course ρ_I is that state and P is a single δ function at q = 0. If there were only two pure states (related by a global flip) [26], then Pwould simply be a sum of two δ functions at $\pm q_{\rm EA}$. But what if infinitely many pure states ρ_J^{α} coexist in ρ_J , with infinitely many overlap values $q_J^{\alpha\beta}$? If the set of overlap values were *countably* infinite, then P_J would necessarily be a sum of δ functions, but the infinitely many locations (as well as the weights) would not depend on J. We regard as implausible such a selection of preferred J-independent values of the overlaps. A plausible alternative for multiple pure states and overlaps is where the countable decomposition Eq. (2) is replaced by an integral and P is continuous.

Ultrametricity.—We briefly turn to the question of whether ultrametricity of pure state overlaps [27] can survive in short-ranged spin glasses, given that P_J is self-averaged. Clearly, this type of nontrivial ultrametricity requires the existence of multiple pure states. As discussed above, we consider the case where P(q) is continuous. We now demonstrate that such an overlap distribution cannot have an ultrametric structure, in the Parisi sense.

Let $\alpha, \beta, \gamma_1, \gamma_2, \ldots$ denote pure states randomly selected from the continuum of such states [according to the integral replacement for Eq. (2)], and let their overlaps as usual be denoted $q^{\alpha\beta}$, etc. In the Parisi solution, these overlaps are such that, for any k, the two smallest of $q^{\alpha\beta}, q^{\alpha\gamma_k}$, and $q^{\beta\gamma_k}$ are equal. For nontrivial ultrametricity such as occurs in the Parisi solution, there would be positive probability that for some i and j the following two strict inequalities occur simultaneously:

$$q^{\alpha\gamma_i} < q^{\beta\gamma_i}$$
 and $q^{\alpha\gamma_j} > q^{\beta\gamma_j}$. (6)

If ultrametricity holds, then the first inequality requires that $q^{\alpha \gamma_i} = q^{\alpha \beta}$, while the second inequality requires that $q^{\beta \gamma_j} = q^{\alpha \beta}$. Thus $q^{\alpha \gamma_i} = q^{\beta \gamma_j}$. But because α , β , γ_i , and γ_j are chosen randomly and independently, the two variables $q^{\alpha \gamma_i} = q^{\beta \gamma_j}$ are also independent. Because each of these is chosen from a *continuous* distribution *P*, the probability that the two overlap values can be identical is zero, and we arrive at a contradiction.

The only way to avoid the contradiction is if the two strict inequalities in Eq. (6) *cannot* occur simultaneously. This means that either $q^{\alpha \gamma_k} \leq q^{\beta \gamma_k}$ for *every* k or vice versa, which implies that the pure states can be ordered into a one-dimensional continuum, and the ultrametric structure resembles a comb rather than the usual tree.

As discussed previously, self-averaging makes it implausible that the set of overlaps is countable. A countable set of overlaps would invalidate the above argument and possibly rescue ultrametricity, but at the cost of destroying anything resembling the Parisi solution.

Decomposition into pure states.—What is the nature of the decomposition of ρ_J into pure states? The possibility of a sum as in Eq. (2) (with a countable infinity of self-averaged $q_J^{\alpha\beta}$'s) has already been ruled out as implausible. Thus, in any reasonable scenario for ρ_J , there should be at most one pair of pure states (related by a global spin flip) with *strictly* positive weight.

In other words, either (a) ρ_I is pure, (b) it is a sum of two pure states related by a global flip, (c) it is an integral over pure states with none having strictly positive weight, or (d) it has one "special" pair of pure states with strictly positive weight and all the rest with zero weight. Case (a) occurs if the system is in a paramagnetic phase, or any other in which the EA order parameter is zero. Case (b) would occur according to the Fisher-Huse droplet picture [15], but could also occur if there existed multiple pure states not appearing in ρ_I ("weak Fisher-Huse") [28]. Case (c) occurs if there are uncountably many pure states in the decomposition of ρ_{I} , all with zero weight ("democratic multiplicity"). Case (d) (which we regard as unlikely) occurs when one pair of pure states partially dominates all others, but accounts for only part of the total weight ("dictatorial multiplicity").

What is the nature of $P (= P_J)$ obtained from ρ_J in the three (nontrivial) cases (b)–(d) discussed above? Clearly case (b) implies that P is a sum of two δ functions at $\pm q_{\rm EA}$, and no continuous part. If we assume in cases (c) and (d) that varying α and β through the continuous portion of the pure states yields a continuously varying $q_{\alpha\beta}$ [but see the next paragraph for an example of case (c) where this assumption is violated because $q_{\alpha\beta}$ does not vary but is fixed at 0], then it follows that case (c) corresponds to a P with no δ functions while case (d) corresponds to a P with δ functions at $\pm q_{\rm EA}$ and a continuous part. This latter case is the P predicted by the Parisi solution, but note two crucial distinctions between case (d) and the SK picture: (i) There is self-averaging, so one already obtains the continuous part of P from a single realization J, and (ii) the δ functions at $\pm q_{\rm EA}$ come from a *single* special pair of pure states—not from countably many $a^{\alpha\alpha}$'s.

We remark that a case of democratic multiplicity occurs in a solution for the ground state structure in a short-ranged, highly disordered spin glass model [29]. We argued there that below eight dimensions, there exists a single pair of ground states [case (b) above], while above eight, there are uncountably many. It is not hard to see that the ρ_J for d > 8 corresponds to case (c) above—the states are chosen by the flips of fair coins for all the trees in the "invasion forest," so all have equal (zero) weight. It appears that for this ρ_J , P(q) is a δ function at zero. This shows that, in general, such a P does not rule out the existence of many states.

In conclusion, we have proved that in short-ranged spin glass models a natural construction leads to a non-self-averaged thermodynamic state ρ_J whose Parisi overlap distribution P_J is translation invariant and hence self-averaged. This demonstrates non-mean-field behavior for realistic spin glasses. The arguments, which are mathematically rigorous, show more generally that translation invariance of P_J is inconsistent with non-self-averaging.

In this paper we have shown that the SK picture in its most straightforward interpretation is incorrect (or at best incomplete). Any thermodynamic theory of realistic spin glasses will differ considerably from this picture. The question then is whether and how any aspects of mean field behavior can survive in such a theory. We will address this issue in a separate paper.

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