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Limits $d \to \infty$ and $T \to 0$ may not commute in the Ising spin glass

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A replica-symmetric low-temperature expansion for the short-range Ising-spin-glass model may be arranged by the number of flipped sites—sites that have spins in some, say m, of the n replicas "down." The contribution of states with up to three flipped sites is obtained for the free energy and the Edwards-Anderson order parameter. The two-flipped-sites contribution to the free energy, which at $d \to \infty$ gives the (negative) zero-temperature entropy of the Sherrington-Kirkpatrick model, is shown at *finite d* to give *no* entropy at $T=0$. Higher-order contributions are argued to also not give any entropy at $T=0$.

Theoretical studies of spin glasses seem to have reached an impasse in the past few years. On the one hand, the Parisi solution[1] to the Sherrington-Kirkpatrick (SK) model[2]—the mean-field solution—predicts many pure states in the spin-glass phase, and the space of these states is ultrametric.[3] The solution was first obtained using the concept of replica symmetry breaking.[1,3] On the other hand, phenomenological scaling theories predict only two pure states.[4,5] The scaling theories are thought to be valid for d-dimensional spin glasses with short-range interactions when d is not much larger than the lower-critical dimension, which is between two and three. Indeed, a scaling theory based on the behavior of the large-scale droplets of low-energy excitations, by Fisher and Huse, has been quite successful in explaining unusual dynamical effects observed in real spin glasses.[6] In spite of these successes, however, there does not exist any detailed theoretical study of a model spin-glass phase in finite dimensions that shows why the mean-field theory predictions are so different from those of the scaling theories. Several further arguments support the scaling-theory predictions;[7] detailed analyses of the spin-glass transition, however, have been carried out only for the approach to the transition from the high-temperature, paramagnetic phase.[8] Even computer simulations, although they have been extremely successful in elucidating the critical behavior at the spin-glass transition in three dimensions,[9] have not provided us an unambiguous answer on the nature of the spin-glass phase in finite-dimensional systems.[10]

Here, we shall discuss a replica-symmetric low-temperature expansion for the d-dimensional Ising spin glass. The expansion shows that the thermodynamic behavior of the excitations about the replica-symmetric ground state is singular in the limit $d \to \infty$. The feature of the expansion that underlies this suggestion: A term in the expansion of the free energy that in the SK limit reproduces the negative zero-temperature entropy of that model but contributes no zero-temperature entropy when it is expanded about $T=0$ at finite d. To appreciate the significance of this result for spin-glass theory, let us recall that the negative zero-temperature entropy of the SK solution was one of the two reasons that motivated the search for solutions with broken replica symmetry. The negative value of the Edwards-Anderson susceptibility was the second reason.[11-14]

We shall discuss the low-temperature expansion for the finite-dimensional Ising-spin-glass model defined by the Hamiltonian[15]

$$H = \tfrac{1}{2} \sum_{i \neq j} J_{ij} \sigma_i \sigma_j \, . \tag{1}$$

Here, σ_i and σ_j are Ising spins at sites i and j and J_{ij} are elements of the random-exchange-interaction matrix between spins on nearest-neighbor sites of a d-dimensional hypercubic lattice. The distribution of J_{ij} is continuous and symmetric about 0, and the variance J^2 is its only nonzero cumulant. In the replica method the thermodynamics of a system with quenched disorder are obtained from the statistical mechanics of an effective Hamiltonian that is derived from the average over the quenched random variables of the nth power of the partition function.[15] The effective Hamiltonian for the problem defined by (1) is

$$[Z^n]_{\rm av} = \operatorname*{Tr}_{s_i^\alpha} \exp(-\beta H_n) \, , \tag{2}$$

$$-\beta H_n = \tfrac{1}{4} \beta^2 \sum_{i \neq j} \left(\sum_{\alpha=1}^{n} s_i^\alpha s_j^\alpha \right)^2 . \tag{3}$$

Thus there is an n-component vector s_i^α, $\alpha = 1, \ldots, n$, at every site i. Each component of this vector is an Ising variable and may be $+1$ or -1.

The description of the spin-glass phase obtained in the scaling theories raises the tantalizing possibility that the short-range spin-glass model (1), when it is reformulated as in (2) and (3), might be replica symmetric. What is the replica-symmetric ground state of (2) and (3)? Unfortunately, there do not seem to be any studies of low-temperature properties of the replicated model (2) about its possible replica-symmetric ground states. This is not all that surprising, in spite of the worldwide interest in the model for the past 15 years, for the following two reasons. First, the notion of replica symmetry and of the breaking of this symmetry first arose in the SK, or mean-field, approximation.[2] In such approximations one usually introduces "collective fields" that are conjugate to the ordering fields, and one looks for nontrivial solutions to the equations of state for the collective fields. In the SK model, the collective fields are the elements $q^{\alpha\beta}$, $\alpha \neq \beta$, of the $n \times n$ matrix of overlaps between different replicas α and β. In the SK solution, which *is* replica symmetric, the $q^{\alpha\beta} = q_{\rm SK}$ are all equal. In the Parisi solution, by contrast, the *permutation* symmetry between different replicas is broken, so that all the $q^{\alpha\beta}$ are not the same. But such a discussion of replica symmetry in terms of elements $q^{\alpha\beta}$ of the order-parameter matrix does not reveal what configuration of the replicated spin variables s_i^α describes the replica-symmetric or replica-symmetry-broken ground state of the model. Second, since a proper understanding of the mean-field theory is regarded as an important first step in the study of phase transitions, the recognition that the replica symmetric solution to the SK model is unstable[11,12] discouraged further thinking on replica-symmetric ground states of the finite-dimensional, short-range model.

The low-temperature expansion we shall discuss for the statistical mechanical problem defined by (2) and (3) was inspired in part by a solution to the renormalization-group equations for kink energies in a one-dimensional model with long-range interactions,[16] and, in part, by the hope raised by the scaling theories that the finite-dimensional Ising spin glass might be replica symmetric. Use of the replica method in Anderson localization, where replica symmetry is unbroken, has shown that results obtained for integer values of n when continued to $n \rightarrow 0$ are meaningful if the theory turns out to be replica symmetric.[17] Indeed, the low-temperature expansion we shall discuss is about a state that maximizes the Boltzmann factor in (2) and (3) for integer n, and the topology, as well as the energies, of excitations about that state have the same form as those of kinks in the solution to the one-dimensional long-range model discussed in Ref. 16.

All spins in all replicas at all sites point in the same, say "up," direction in the state about which we shall discuss the low-temperature expansion. So the expansion may be arranged by the number of flipped sites—sites with "down" spins in some, say m, of the n replicas. I have calculated contributions to the equation for the order parameter q (see below for a precise definition), as well as to the free energy, from states with up to three flipped sites. All these reduce in the SK limit—the limit $d \rightarrow \infty$ when $J^2 \sim 1/d$—to expressions familiar in the SK solution. For example, the expansion for the order parameter matches the first three terms in the series obtained by iterating about $q_{\rm SK} = 1$ the self-consistent equation for the order parameter $q_{\rm SK}$ in the SK solution. This similarity is evidence that the expansion is about the ground state described by the nonzero value of the replica-symmetric, or SK, ansatz for the order parameter matrix $q^{\alpha\beta}$.

Let us first discuss the choice of the ground state in a little more detail, and then turn to contributions to the free energy—especially, the two-flipped-sites contribution, which in the SK limit gives the negative zero-temperature entropy of the SK solution. For the problem defined by (2) and (3) the Boltzmann factor is maximum for states in which $s_i^\alpha = s_j^\alpha$. These are states in which each replica is independently ferromagnetically aligned throughout the system. The states are 2^n-fold degenerate. But the Edwards-Anderson (EA) order parameter is zero when averaged over these states. To see this let us follow De Dominicis and Young[18] and define the EA order parameter q as

$$q = \lim_{n \rightarrow 0} \frac{1}{n(n-1)} \sum_{\alpha \neq \beta}^{n} \langle s_i^\alpha s_i^\beta \rangle .$$

Then, in a state with m_1 down spins at each site,

$$\sum_{\alpha \neq \beta}^{n} s_i^\alpha s_i^\beta = (n - 2m_1)^2 - n .$$

Summing over m_1 because states with different m_1 have the same energy, and using binomial weights $\binom{n}{m_1}$ for different m_1 values, we get 0, because

$$\sum_{m_1=0}^{n} \binom{n}{m_1} (n - 2m_1)^2 = n .$$

This result is not surprising, because we know that when carrying out an expansion of the partition function about a state that breaks the symmetry of the Hamiltonian, we must introduce a small symmetry-breaking field to stabilize the broken-symmetry state. In the Ising ferromagnet, for example, a uniform field must be applied to pick out one of the two possible ground states—those are the state with all spins up and the one with all spins down. For the replica-symmetric solution, the symmetry-breaking field is thought to be a Gaussian random variable.[13] Such a field adds a term of the form

$$\sum_{i, \alpha \neq \beta} s_i^\alpha s_i^\beta$$

to the Hamiltonian in (3). The effect of this term is to align the replicas at *each* site. We shall not keep this "field" term explicitly in the Hamiltonian, but we shall choose the state favored by this term as our ground state. This is the state in which spins in all replicas at each site point up.

The energy of the ground state is of order n^2, so its contribution to the free energy vanishes in the limit $n \rightarrow 0$. For each flipped site we must sum over the $2^n - 1$ states that that site may be in if it is not in the ground state. We may write the free energy per site as

$$f = f_1 + d f_2 + d(2d-1) f_3 \cdots \tag{4}$$

where the d-dependent prefactors of f_r's give the number of ways per site for choosing a connected cluster of r-flipped sites on a d-dimensional hypercubic lattice.[19] Unlike the Ising model or other spin models, many-spin-flipped states contribute to the free energy of the model (2) and (3) only when the flipped sites form a connected cluster. This is true also for the contributions to the EA order parameter. The fact that each connected cluster gives a contribution of order n to the free energy is the reason for this feature of the expansion. So when the contributions of configurations consisting of disconnected clusters are divided by n, the result for the free energy varies as a positive power of n—one less than the number of connected clusters—and vanishes when the limit $n \rightarrow 0$ is taken.

The expression for f_1 was given in Ref. 16; it is the same as obtained when $q_{\rm SK}$ is set equal to unity in the SK free energy. The procedure outlined above gives for f_2,

$$-\beta f_2 = \int [dy_1][dy_2][dy_{12}]\ln[\Phi_2] - \int [dy_1][dy_{12}]\ln[2\cosh(J\beta y_1 + J\beta y_{12})] - \int [dy_2][dy_{12}]\ln[2\cosh(J\beta y_2 + J\beta y_{12})], \quad (5)$$

where

$$\Phi_2 = 4\cosh(J\beta y_1)\cosh(J\beta y_2)\cosh(J\beta y_{12}) + 4\sinh(J\beta y_1)\sinh(J\beta y_2)\sinh(J\beta y_{12}). \quad (5a)$$

The integrals have Gaussian weight factors—of variance $(2d-1)/2$ for y_1 and y_2 and of variance $\frac{1}{2}$ for y_{12}. That is

$$\int [dy_{1,2}] \equiv \int_{-\infty}^{+\infty} \frac{dy_{1,2}}{[\pi(2d-1)]^{1/2}} \exp[-y_{1,2}^2/(2d-1)].$$

To compare this to the SK solution, let $J = \tilde{J}/\sqrt{d}$ and take the limit $d \to \infty$, which gives

$$f_2^\infty \equiv \lim_{d\to\infty} df_2 = \frac{1}{4}\beta\tilde{J}^2\left(1 - \int [dy] M_1(\beta\tilde{J}y)^2\right)^2. \quad (6)$$

The notation $M_r(y) = d^r M_0(y)/dy^r$ and $M_0(y) \equiv \ln(2\cosh y)$ is familiar in the series analysis of the Ising model: $M_r(y)$ are cumulants of an isolated Ising spin in a magnetic field y/T.[20] The expression for f_2^∞ is the same as obtained when once-iterated q_{SK} is substituted in the SK free energy, and it gives a value of $-1/2\pi$ for the zero-temperature entropy.

At finite d, the large-β—or low-temperature—expansion for f_2 is of the form

$$-\beta f_2 = \beta f_{2,-1} + (1/\beta) f_{2,1},$$
$$f_{2,-1} = (4/\pi^{3/2})([(2d-1)/2]^{1/2}\cot^{-1}\{[(2d-1)/2]^{1/2}\} - (2d)^{1/2}\cot^{-1}[(2d)^{1/2}]), \quad (7)$$
$$f_{2,1} = (4/\pi^{3/2})\eta(2)(1/4[(2d-1)/2]^{-1/2}\cot^{-1}\{[(2d-1)/2]^{1/2}\} + (2d)^{-1/2}\cot^{-1}[(2d)^{-1/2}]) + (1/2\pi d)^{1/2}\eta(2),$$

where

$$\eta(s) = \sum_{m=1}^{\infty} -(-1/m)^s.$$

The exact values of the coefficients in the expansion (7) is not of interest right now; that the expansion has no constant term is of interest, because it implies that the entropy vanishes at $T=0$.

The three-flipped-sites contribution to the free energy f_3, as well as the four-flipped-sites contribution when the four flipped sites lie on the vertices of a square, are similar to f_2. The former involves a five-dimensional integral, with Gaussian weights, of a logarithm of a sum of products of exponential factors (which may be written as a sum of products of hyperbolic functions); the latter involves an eight-dimensional integral. The logarithms in each case arise from continuing to $n \to 0$ the nth power of multinomials of products of exponential factors. These results suggest very strongly that the higher-order contributions all involve similar multiple Gaussian integrals of logarithms of sums of products of exponential factors. (Details about higher-order terms—from connected clusters of four or more flipped sites—as well as their contribution to the order parameter, will be published separately.) It is therefore instructive to briefly review the mathematical steps taken to obtain the large-β expansion (7) for f_2, for it seems that the higher-order terms will also not give any nonzero contribution to the entropy at $T=0$.

It is best to write out the integrand in (5) separately in each quadrant or octant and to restrict the ranges of integration to positive line segments. In quadrants or octants in which all or an even number of the variables are positive, the large-β expansion is quite straightforward and is obtained by a procedure similar to the one used for expanding the SK free energy around $T=0$: After factoring out a symmetric product of exponential factors, the argument of the logarithm is one plus a sum of products of exponential factors of *negative* arguments. So the logarithm may be expanded because each exponential is small for large β. Each term in the expansion now involves integration of exponentials of quadratic functions over semi-infinite positive line segments. Each such integration yields an error function of argument proportional to β, for which the asymptotic series for large β starts at $1/\beta$ and has no term independent of β.

In quadrants or octants in which all or an odd number of variables are negative, it is not possible to write the argument of the logarithm as one plus a sum of exponentially small factors—the argument *is* a sum of exponentially small factors. So one must break the volume of integration into simplexes in each of which the variables are ordered by magnitude. The procedure outlined above may now be used for each simplex. But the large-β behavior is more difficult to extract because the ranges of integration are now finite. Each integration step may still be expressed as an integral or repeated integral of some error function or as an incomplete γ function of arguments proportional to β. All these functions have asymptotic expansions for large β that start at $1/\beta$ and do not have the constant term.

The perceived similarity of the higher-order contributions to those of two-, three-, and (one of the) four-flipped-site contributions, and the analytical properties of these contributions outlined above when discussing their large-β expansions, suggest *very* strongly that in the replica-symmetric expansion discussed here the entropy vanishes at $T=0$ for all finite d, quite unlike the result obtained by SK by taking the limit $d \to \infty$ *before* expanding the thermodynamic properties about $T=0$.

As already mentioned, a negative value of the $T=0$ entropy in the mean-field, SK solution was one of the two reasons that motivated the search for mean-field solutions with broken replica symmetry. So the above discussion on the vanishing of the $T=0$ entropy in the replica-symmetric spin-glass phase at finite d brings us a step closer to resolving whether the ground state of the short-range Ising-spin-glass model is replica symmetric or whether it too breaks replica symmetry. Final resolution of this puzzle must await a careful examination of the Edwards-Anderson susceptibility, for proof of the non-negative value of this susceptibility was an important criterion for the acceptance of the Parisi solution even after there was reason to believe that the zero-temperature entropy vanished in that solution.[13,14]

It would be of interest to carry out the low-temperature expansion outlined here also for the model defined on the Bethe lattice, as well as for other mean-field-like Ising-spin-glass models with finite connectivity.[21] Finally, one might also like to compare the energy of the replica-symmetric ground state discussed here against possible replica-symmetry-broken ground states. It is heartening to note in this regard that the p-adic analysis of replica symmetry breaking[22] might make it possible to develop a low-temperature expansion for the Parisi solution at finite d, and therefore to compare at finite d the ground-state energy in that solution with that in the replica-symmetric solution.

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