Zero-Temperature Entropy of a Replica-Symmetrical Spin-Glass

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Zero-temperature entropy of a replica-symmetric spin glass

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An exact expansion is obtained for the free energy of the Ising spin glass with an arbitrary distribution of exchange bonds when the ground state is assumed to be replica symmetric. The expansion is examined for low-temperature thermodynamics. It is argued that the zero-temperature entropy is zero for a bimodal distribution of exchange bonds if the distribution has an infinitesimally small asymmetry.

Identification of the low-energy defects in an ordered phase provides interesting insights into the nature of that phase.[1] And good estimates of the energy (or free-energy) cost of creating those defects provide a point of departure for developing detailed, quantitative theories for the stability of the phase and for the phase transitions by which the phase is obtained.

In this paper I shall discuss in the context of the replica formalism the nature of defects in the *replica-symmetric* Ising spin glass.[2] I shall present an expansion for the free energy in the number of defects.[2] The expansion leads to the conclusion that the zero-temperature entropy of the replica-symmetric Ising spin glass is zero at all finite dimensions when the random-bond distribution is bimodal and has an infinitesimally small value for the mean. By contrast, the zero-temperature entropy is negative for all distributions, including the asymmetric bimodal distribution, when $d \rightarrow \infty$ and the cumulants of the distribution are suitably scaled by powers of $1/d$ to obtain a finite free energy.

The value of the zero-temperature entropy has been of great concern in spin-glass theory ever since the paper by Sherrington and Kirkpatrick[3] (SK) in 1975, which presented a precise formulation of the ideas in a paper by Edwards and Anderson.[4] The SK paper showed that a simple ansatz for the saddle point giving the mean-field description of the Ising spin glass, called the replica-symmetric ansatz, leads to a negative value of the zero-temperature entropy. That saddle point is unacceptable for another reason: In 1978 de Almeida and Thouless showed that the spectrum of fluctuations about that saddle point has an unstable mode.[5] It took almost 5 years before a physically acceptable saddle point was discovered, by Parisi, by breaking the replica symmetry in a specific way.[2]

Is the spin-glass phase in $d=3$—or, for that matter, at any finite d—similar to the phase discovered by Parisi in the context of mean-field theory? The question has not been resolved yet, although De Dominicis and Kondor have made considerable progress in studying fluctuations about Parisi's mean-field theory.[6] Meanwhile, the question's relevance now extends far beyond the need to understand the low-temperature behavior of dilute magnetic alloys, because ideas developed to understand replica-symmetry breaking have found applications in a variety of fields.[2,7] In the absence of any definitive study of the possible spin-glass phase or *phases* at finite d, however, a variety of arguments have accumulated suggesting that for the Ising spin glass, unlike the ferromagnet or any other widely discussed ordered phase, the mean-field theory may be a singular limit of the models as a function of the dimensionality.[8,9]

The result about the vanishing of the zero-temperature entropy of a replica-symmetric spin glass is not sufficient to decide the important question about the nature of the spin-glass phase at finite d, namely, whether or not it is replica symmetric. Settling that question will require studies of the Edwards-Anderson susceptibility, which is inversely related to an eigenmode of the replica theory that is unstable in the replica-symmetric choice of the mean-field saddle point.[10] Comparison between the ground-state energies of the replica-symmetric and possible replica-symmetry-broken phases may also be necessary in settling that question.[11] But the result about the zero-temperature entropy in the replica-symmetric phase at finite d is important for at least three reasons. First, it is an exact result. Second, it provides the first concrete hint for the possibility that the spin-glass thermodynamics at finite d might *indeed* be very different from those at $d \rightarrow \infty$. Third, it underscores once again the need to study the Ising spin glass in finite dimensions rather than by expansions about the mean-field theory.[12]

It should also be mentioned in passing that the fact the result for the zero-temperature entropy discussed here is for a bimodal distribution, rather than for the Gaussian, which is more often studied analytically, is an advantage rather than a drawback. This is because a lot of numerical work, especially the extensive searches by Sourlas for thermodynamic behavior indicative of replica-symmetry breaking,[13] has been done predominantly for a bimodal distribution.

Let us start with the usual Ising spin-glass model[2–4] defined by the Hamiltonian

$$H = \sum_{(i \neq j)} J_{ij} \sigma_i \sigma_j \ . \tag{1}$$

Here σ_i and σ_j are Ising spins at sites i and j, and J_{ij} are random exchange bonds between spins on nearest-neighbor sites of a d-dimensional hypercubic lattice. The sum is over all distinct nearest-neighbor pairs (ij). Let the distribution $P(J_{ij})$ of each J_{ij} be defined by the cumulants J_m, $m>0$. 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.[4] Using the definition of cumulants, the effective Hamiltonian for the problem defined by (1) is

$$(Z^n)_{\text{av}} = \operatorname*{Tr}_{\sigma_i^\alpha} \exp(-\beta H_n) \ , \tag{2}$$

$$-\beta H_n = \sum_{(i\neq j)} \sum_{m=1}^{\infty} \frac{J_m}{m!} \left[\beta \sum_{\alpha=1}^{n} \sigma_i^\alpha \sigma_j^\alpha \right]^m . \tag{3}$$

Thus there is an n-component vector σ_i^α, $\alpha=1,\ldots,n$, at every site i. Each component of the vector is an Ising variable and takes values $+1$ or -1.

Following the successful use of the replica method in Anderson localization, where replica symmetry is unbroken, we may in our study of the replica-symmetric spin-glass phase treat σ_i^α as if we had an integer number of Ising spins and disregard any complications that might arise from the limit $n\to 0$, which we must take in the end. We therefore regard as our ground state the state that maximizes $-H_n$ and in which the Edwards-Anderson (EA) order parameter, defined by De Dominicis and Young as[14]

$$q = \lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta}^{n} \langle S_i^\alpha S_i^\beta \rangle \ , \tag{4}$$

is unity. This is the state in which all replicas at each site point in the same, say, "up," direction.[9] Excitations about this ground state consist of sites (or contiguous clusters of sites) at which spins in some of the n replicas point down. (We shall call sites having spins in some of the replicas misaligned with respect to the ground state "flipped sites," and we shall call replicas misaligned with respect to the ground state "flipped replicas.") To obtain the contribution of these excitations to the free energy, one must sum the number of flipped replicas between 1 and n at each flipped site. Furthermore, because the replicas are all regarded as equivalent, states with different numbers of flipped replicas must be weighted by binomial coefficients, which give the number of ways of partitioning the set of n replicas into subsets of aligned and misaligned replicas.

In this description of the states of the "replicated" Ising spin-glass model, there is a kink-like defect in the lattice whenever two nearest-neighbor sites have spins in one or more replicas pointing in opposite directions. These kinks satisfy the renormalization-group equation for kink couplings in a one-dimensional random-exchange Ising model with power-law interactions.[15]

For the Gaussian distribution of exchange bonds, the contribution of states with a few flipped sites reproduces in the limit $d\to\infty$ the low-temperature expansion for the SK free energy,[9] a fact that should further assure us that the replica-symmetric phase we are studying is the same as obtained and studied in the SK model by the replica-symmetric ansatz for the saddle point.

The free energy, other thermodynamic functions, and the order parameter may now be expanded in the number of flipped sites. The expansion should be reminiscent of the so-called low-temperature expansion for Ising and Heisenberg models. There is, however, a difference. Unlike in pure Ising magnets, for which each term of the expansion is exponentially small at low temperatures, the low-temperature behavior of the terms in the spin glass depends on the form of the probability distribution of exchange bonds.

For a given number p of flipped sites, there may be several topologically distinct clusters, and so the expansion for the free energy per site f may be formally written as

$$f = \sum_{p,r} L_{p,r} f_{p,r} \ . \tag{5}$$

In (5), $f_{p,r}$ is the free-energy contribution of the rth topologically distinct connected cluster of p flipped sites and $L_{p,r}$, the lattice factor, is the number of ways per site of obtaining that connected cluster of p sites. The lattice factors may be obtained from the known low-temperature expansion for the Ising ferromagnet.

Unlike the use of the low-temperature expansions for the Ising ferromagnet, the immediate goal in the study of the Ising spin glass is not to determine the singularities at the spin-glass transition, but to understand the low-temperature thermodynamics around, and stability of, possible spin-glass ground states. For that purpose the expansion (5) may be regarded as exactly known. This is because it is possible to write down a simple rule for obtaining the $f_{p,r}$:

$$f_{p,r} = (-1/\beta)\Phi_{p,r} - \sum_{s=1}^{p-1} \sum_{l} C_{s,l;p,r} f_{s,l} \ . \tag{6}$$

Here $\Phi_{p,r}$ is $-\beta$ times the free energy of the rth topologically distinct cluster of p Ising spins embedded in a lattice of "up" spins and interacting with one another as well as with the lattice of "up" spins with nearest-neighbor random bonds whose distribution, independent for each bond, is given by the cumulants J_m. The partition function $Z_{p,r}$ of the cluster is a function of $R(p,r)$ exchange bonds, hereafter called the flipped bonds y_j, connecting the spins in the cluster to one another and to the lattice of up spins. More precisely, the partition function $Z_{p,r}\{y_k\}$ of the cluster is a sum of 2^p exponentials, one for each of the 2^p states of the cluster of p Ising spins, whose arguments are linear combinations of the y_j's. Formally, the free energy $\Phi_{p,r}$ of the cluster may be written as

$$\Phi_{p,r} = \int \prod_{j=1}^{R(p,r)} dy_j P(y_j) \ln Z_{p,r}\{y_k\} \ . \tag{7}$$

Finally, in Eq. (6), $C_{s,l;p,r}$ is the number of ways the lth topologically distinct *connected* cluster of s flipped sites can be obtained from the original cluster of p flipped sites. For $p=4$, for example, there are two topologically distinct clusters—a chain and a ring. Call them 1 and 2, respectively. Each of these gives rise to a topologically distinct connected cluster with three, two, or one sites, and each of these smaller clusters can be obtained from the original four-site cluster in four ways. Therefore, $C_{3,1;4,1}=C_{2,1;4,1}=C_{1,1;4,1}=4$ for the four-site chain, and the same holds also for the second four-site cluster, the ring.

When the bond distribution is a Gaussian, the case that is more often studied analytically, the number of integrals on the right-hand side of (7) can be reduced by using the property that the distribution of a sum of Gaussian random variables is also a Gaussian random variable.

As an example of how (6) and (7) arise for an arbitrary distribution P, let us consider the contribution of states with one flipped site. (For the Gaussian distribution, this contribution was first discussed in Ref. 15.) The flipped site causes $2d$ flipped bonds, and let the number of flipped replicas be n_1. Therefore, the "Boltzmann" factor is

$$\exp\left[2d\sum_{m=1}^{\infty}\frac{J_m}{m!}[\beta(n-2n_1)]^m\right],$$

and as discussed earlier, we need to sum on n_1 from 1 to n. The sum could be easily carried out if the exponent were a linear function of $n-2n_1$. In the Gaussian case the exponent is easily linearized using properties of Gaussian integrals; for the general distribution discussed here, the linearization may be done using an auxiliary variable λ_j for each flipped bond y_j, which gives

$$\int_{-\infty}^{+\infty}\prod_{j=1}^{2d}dy_j d\lambda_j \exp\left[\sum_{j=1}^{2d}\sum_{m=1}^{\infty}\frac{J_m}{m!}(\lambda_j)^m\right]\sum_{n_1=1}^{n}\begin{bmatrix} n \\ n_1\end{bmatrix}\exp\left[i\sum_{j=1}^{2d}y_j[\lambda_j-(n-2n_1)\beta]\right] \tag{8}$$

$$=\int_{-\infty}^{+\infty}\prod_{j=1}^{2d}dy_j d\lambda_j \exp\left[\sum_{j=1}^{2d}\sum_{m=1}^{\infty}\frac{J_m}{m!}(\lambda_j)^m\right]\exp\left[i\sum_{j=1}^{2d}y_j\lambda_j\right]\left\{\left[2\cosh\left[\beta\sum_{j=1}^{2d}y_j\right]\right]^n-1\right\}. \tag{9}$$

The coefficient of the term linear in n, needed for the limit $n\rightarrow 0$, is logarithm of the cosh in (9). We may once again use the definition of the cumulants to write (9) as

$$\int_{-\infty}^{+\infty}\prod_{j=1}^{2d}dy_j P(y_j)\ln\left[2\cosh\left[\beta\sum_{j=1}^{2d}y_j\right]\right]. \tag{10}$$

Equations (5)–(7) were obtained by generalizing the result obtained by carrying out for several clusters calculations such as the one outlined above for one flipped site. Results for up to three flipped sites have already been discussed in Ref. 9 for the Gaussian distribution. But the generalization to arbitrary cluster size and distribution summed up in Eqs. (5)–(7) above allow us to infer without further calculation the behavior of the zero-temperature entropy for the asymmetric bimodal distribution.

It should be apparent from an inspection of Eqs. (5)–(7) that the free energy for finite d will be a linear combination of logarithms when the distribution P is discrete and consists of a sum of a finite number of δ functions. The arguments of the logarithms will be sums of exponentials of arguments proportional to β. To extract the low-temperature—or large-β—behavior of the free energy, we may factor out the exponential with the largest exponent. The logarithm of it, being proportional to β, will give a contribution to the ground-state energy. The rest of the free energy will consist of a linear combination of logarithms of arguments 1 plus, at low temperatures, exponentially small factors. This suggests that the zero-temperature entropy will be zero.

Unfortunately, there is a weak link in the argument of the previous paragraph. Consider, for example, a symmetrical bimodal distribution, in which the bonds take values $+J$ or $-J$ with equal probability. When an even number of random variables with such a distribution are added, the distribution of their sum has a nonzero weight at value zero. This observation shows that the arguments of logarithms in Eq. (7) may be pure numbers. The observation therefore invalidates, for terms arising from an even number of flipped bonds, the claim in the previous paragraph that arguments of the logarithms are sums of exponentials. Some preliminary results show that such terms add up to zero. There is, fortunately, an alternative way to circumvent this difficulty. If we start with a bimodal bond distribution that has an infinitesimally small asymmetry—with δ functions at $J+\epsilon$ and $-J+\epsilon$, with ϵ infinitesimal—then the distribution of the sum of any number of such bonds will not have a nonzero weight at a value of the sum equal to zero. For such a distribution, then, the zero-temperature entropy of the replica-symmetric phase of the Ising spin glass is zero at finite d.[16]

The zero-temperature phase diagram of the Ising spin glass with an asymmetric distribution has both a spin-glass phase and a ferromagnetic (or antiferromagnetic, depending on the sign of the mean) phase. In mean-field theory the ferromagnetic or antiferromagnetic phase sets in when the value of the mean is of the same order but bigger than the variance. This must be true also in finite dimensions. We can therefore be sure that the result about the zero-temperature entropy obtained above is valid in the spin-glass phase, because the mean ϵ was assumed to be infinitesimally small.

The low-temperature behavior obtained above contrasts sharply with that obtained in the limit $d\rightarrow\infty$. In that case even discrete distributions reduce to a Gaussian or a Gaussian multiplied by a polynomial, depending on the order in $1/d$. In particular, the two-flipped site term, which was identified in Ref. 9 as the cause of the negative value of the zero-temperature entropy of the replica-symmetric SK solution, gives a negative value for the zero-temperature entropy for all distributions in the limit $d \rightarrow \infty$. And as in the Gaussian case, terms arising from more-than-two flipped sites do not contribute to the zero-temperature entropy at $d \rightarrow \infty$ for any symmetric distribution of the exchange bonds.

It would be interesting to use the ideas discussed here to develop a quantitative theory for the phase transition in the random-field Ising model.

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[1]See, for example, P. W. Anderson, *Basic Notations of Condensed Matter Physics* (Benjamin-Cummings, Menlo Park, CA, 1984), Chap. 2.

[2]For an introduction as well as an extensive discussion of replica symmetry and the breaking of this symmetry, see M. Mezard, G. Parisi, and M. A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987).

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[5]J. R. L. de Almeida and D. J. Thouless, J. Phys. A **11**, 983 (1978). See also E. Pytte and J. Rudnick, Phys. Rev. B **19**, 3603 (1979); A. Khurana and J. A. Hertz, J. Phys. C **13**, 2715 (1980).

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[7]For a brief but insightful discussion of the applications of spin-glass ideas, see P. W. Anderson, Phys. Today **42**(9), 9 (1989); **43**(3), 9 (1990).

[8]The arguments include consideration of pure states in Ising systems [D. S. Fisher and D. A. Huse, J. Phys. A **20**, L1005 (1987)]; phenomenological scaling theories [D. S. Fisher and D. A. Huse, Phys. Rev. Lett. **56**, 1601 (1986)]; Phys. Rev. B **38**, 386 (1988); A. J. Bray and M. A. Moore, in *Colloqium on Glassy Heidelberg Dynamics*, Vol. 275 of *Lecture Notes in Physics,* edited by J. L. van Hemmen and I. Morgenstern (Springer-Verlag, New York, 1987); heuristic picture of the spin-glass phase [A. Bovier and J. Frohlich, J. Stat. Phys. **44**, 347 (1986)]. Studies of the correlation matrix support the possibility of unusual behavior in the limit $d \rightarrow \infty$ [A. Khurana, Phys. Rev. B **40**, 9279 (1989)].

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[10]For proof of the acceptable behavior of the replicon mode in the Parisi solution, see D. J. Thouless, J. R. L. de Almedia, and J. M. Kosterlitz, J. Phys. C **13**, 3272 (1980); C. De Dominicis and I. Kondor, Phys. Rev. B **27**, 606 (1983); A. Khurana, J. Phys. **66**, 2843 (1983).

[11]In the mean-field theory, the ground-state energy of the Parisi solution is actually higher than that of the replica-symmetric SK solution. But this is acceptable because the lower-energy solution has a negative value for the zero-temperature entropy and unacceptable behavior of the EA susceptibility.

[12]It is instructive to recall here that of the three paradigms of disordered solids that have been extensively studied in the past 15 years—namely, Anderson localization, the random-field Ising model, and the Ising spin glass—a formalism for studying the critical behavior has been developed only for the mobility edge in Anderson localization, and that formalism involves an expansion about the *lower* critical dimension [F. J. Wegner, Z. Phys. B **35**, 207 (1979).] Moreover, the long, theoretical controversy about the lower critical dimension of the random-field Ising model arose in part from the failure of the expansion about the upper critical dimension (which is 6) to make reliable predictions about the behavior near the lower critical dimension (which is 2). [See, for example, G. Grinstein, J. Appl. Phys. **55**, 2371 (1984).] Therefore, the connection between understanding the nature of defects and developing expansions about the lower critical dimension—used, for example, to obtain the spin-wave renormalization group for the many-component Heisenberg model in $2+\epsilon$ dimensions—must be regarded especially seriously in the study of the spin glass.

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[14]C. De Dominicis and A. P. Young, J. Phys. A **16**, 2063 (1983).

[15]G. Kotliar, P. W. Anderson, and D. L. Stein, Phys. Rev. B **27**, 602 (1983); A. Khurana, Phys. Rev. B **40**, 2602 (1989). The "pure" counterparts of similar models have been extremely useful in elucidatinng the pure magnets' phases and phase transitions near their lower critical dimensions.

[16]It is common to make the bimodal distribution asymmetrical by changing the relative weights of the two symmetrically placed δ functions, but the form discussed in the text is simpler because its only odd nonzero cumulant is the mean.