Generating low-temperature expansions for Ising spin glasses

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We define a prescription to generate the low-temperature expansion of the free energy of the Ising spin glass. We test our ideas by computing the first few coefficients in $D=2$. Our results indicate that the series coefficients are not numbers but averages over a nontrivial distribution.

Studies of spin glasses[1] are predominantly Monte Carlo simulations.[2] Whereas high-temperature expansions exist for Ising spin glasses,[3] low-temperature expansions have been unavailable for spin glasses because it has not been clear how to define such an expansion in view of the complicated vacuum structure and the quenched averaging that is necessary.

In a recent paper, we studied these systems by generating their partition functions exactly on small lattices and studying their zeros.[4] In the present paper, we use these partition functions in a new way to define and compute the low-temperature expansion for the free energy in the thermodynamic limit.

Starting from general arguments, we first determine a prescription to compute the coefficients of such an expansion. This is described in Sec. I. In Sec. II, we test our scheme in $D=2$ and estimate a few expansion coefficients in the thermodynamic limit. We end with some general remarks and a summary of our results

I. GENERAL CONSIDERATIONS

The Ising spin glass is defined by the Hamiltonian,

$$H_J(\sigma) = \sum_{\langle i,j \rangle} \frac{1}{2}[1 - \sigma_i J_{ij} \sigma_j] , \tag{1.1}$$

where σ_i has the values ± 1, $\langle i,j \rangle$ denotes all nearest-neighbor pairs of sites on the lattice and for each such pair, the energy term depends on the bond J_{ij} which can be ± 1. The free energy is defined as a "quenched average" over all bond configurations. Thus

$$F(\beta) = \sum_J F_J(\beta) \Big/ \sum_J , \tag{1.2}$$

where

$$F_J(\beta) = \ln[Z_J(\beta)]/V , \tag{1.3}$$

and

$$Z_J(\beta) = \sum_\sigma \exp[-\beta H_J(\sigma)] \tag{1.4}$$

is the partition function for a fixed bond configuration.

Since σ_i are bivalued, we can think of them as bit variables. Assuming a certain ordering of the lattice sites, the σ_i for a given lattice configuration can be represented by an integer σ ranging from 0 to $2^V - 1$, where V is the volume. A useful measure of the distance between two lattice configurations σ and σ' is the bit distance, defined as the number of bits that are different in the integers σ and σ'.

Since H_J takes on discrete values, for finite systems, Z_J is a finite polynomial in $u = e^{-\beta}$. Let D be the dimension. Then

$$Z_J = \sum_{i=0}^{DV} q_i u^i = q_0 \sum_{i=0}^{DV} p_i u^i . \tag{1.5}$$

The summation index i is just a count over the discrete set of values of H_J. Expanding F_J in u defines the low-temperature series. Thus

$$F_J = \ln Z_J / V = \ln q_0 / V + \sum_{i=1}^{\infty} a_i u^i , \tag{1.6}$$

where the a_i's can be expressed in terms of the p_i's.

For each bond configuration, we get a set of a_i values. The low-temperature series for F in (1.2) is defined by averaging these over all bond configurations. Thus

$$F(u) = F_0 + \sum_{i=1}^{\infty} A_i u^i , \tag{1.7}$$

where F_0 is an irrelevant constant and the A's are averages of the a's over bond configurations. Note that F_0 is irrelevant not in the sense that it is without physical content but rather that it is irrelevant to the issue of defining a low-T expansion. Thus

$$A_i = \langle a_i \rangle \tag{1.8}$$

with $\langle \ \rangle$ denoting bond averaging.

We will address two issues here. The first is how to compute the coefficients p_i and a_i in the thermodynamic limit from exact calculations on finite systems. The

second is whether the thermodynamic distribution of the a's is a δ function or not. This would determine whether the A's are numbers or averages over a distribution in the thermodynamic limit.

Let us consider how to compute the p_i's for a fixed bond configuration. We know that the system defined by (1.1) has a number of degenerate vacua. Because of these, there arise several issues that are special to the spin glass which we clarify below.

We begin by considering the case of a simple Ising model with all the bonds set to $+1$. There are two ground states, one with all the $\sigma_i = +1$ and the other with $\sigma_i = -1$. To compute the low-temperature series one usually expands around a fixed vacuum. However, image that on a finite lattice one enumerated all states and computed the energies of each of them. How would one use this information to generate the low-temperature expansion? The procedure which generalizes to the spin-glass case is as follows: Classify the states with respect to their energy and their bit distance from each ground state. One can then consider two towers of states, one tower for each ground state. A state belongs to a given tower if its bit distance from the vacuum state under the tower is smaller than its bit distance from the other vacuum state. The states in each tower are then classified with respect to the energy and one computes the series for each tower separately. The final result is obtained by averaging the series for the two towers. In the Ising case, this procedure splits the states into two sets, one set over each tower. The series one gets from the two towers are identical. Because of this equality of series over the towers, one never considers the Ising expansion in this way—one just constructs the series on one of the vacua.

For the spin glass, the situation is different. There are a great many ground states and it is not at all clear, a priori, which ground state to build the series on. The only reasonable definition is to compute the series over all ground states and average over all of them. This leads to the following procedure:

(1) Determine all the ground states σ_0^i and all the excited states σ and their energies by explicit enumeration for a fixed bond configuration. The index i labels the ground states.

(2) Find the bit distances $k(\sigma_0^i, \sigma)$ for all excited states σ relative to all the ground states σ_0^i. One can think of k as a "relative" magnetization of the state σ relative to the ground state σ_0^i. We now define a tower of states over each ground state as follows: assign the state σ to the tower of the ground state σ_0^i for which $k(\sigma, \sigma_0^i)$ is the smallest over all i. If the minimum value of k for some state σ is degenerate (i.e., has the same value for several ground states), we assign that state to all the towers.

(3) Now we consider the ground states and their towers one by one. The states in each tower are labeled by their energy $H_J(\sigma)$ and their relative magnetization k. We now define a series for the p_i's in a variable $v = e^{-h}$. Thus

$$p_i = \sum_k p_{ik} v^k . \qquad (1.9)$$

Each state of energy i and relative magnetization k contributes a count of 1 to the coefficient p_{ik} for the tower.

In this way, we generate a double series in u and v for Z_J for each tower. Here h is the "conjugate" field that couples to k.

(4) The final series for Z_J for a given bond configuration is the average overall the series obtained from the towers.

(5) Steps 1–4 are repeated for all the bond configurations.

Several points need to be clarified.

For fixed J, why do we chose to average Z_J and not $\ln[Z_J]$ over the ground states? A priori, there is no reason to choose one over the other. For the lowest-order terms (p_{21}, p_{22}, p_{41}, etc.) which we are concerned with in this paper, it does not matter if we choose to average Z_J or $\ln[Z_J]$. Higher-order terms will depend on which of the two are averaged.

Next, we would like to discuss the need for the relative magnetization k. Without introduction it and its conjugate field, the coefficients Va_i would not have been proportional to the volume. This has to do with (a) the fact that states with an arbitrary number of spins flipped can have arbitrarily small energy relative to the ground state and (b) the fact that the ground states are separated by a finite number of flipped spins. The introduction of an appropriate conjugate field classifies the states in the correct way and eliminates the double counting that would otherwise have happened.

Note that there is no intrinsic meaning to the conjugate field—its meaning is limited to the ground states for a given bond configuration. The field is an artifact to separate the ground states to define a perturbative tower over each ground state. It has to be taken to zero ($v = 1$) after intensive quantities (such as the free energy per site) are obtained.

There is a simple analogy with the $D = 1$ Ising model that further clarifies this issue. Consider the low-temperature expansion of the $D = 1$ Ising model on a finite lattice of L sites with free boundary conditions. It is easy to see that $a_1 = 0$ (except for boundary effects which vanish in the thermodynamic limit). The coefficient a_2 is the number of states N_2 of energy $E = 2$ divided by the volume L. Unfortunately, $N_2 \sim L^2$ and so a_2 diverges as $L \to \infty$. The reason $N_2 \sim L^2$ is that one can get $E = 2$ with one spin flipped, or with two adjacent spins flipped, or with three adjacent spins flipped, and so on up to $L - 2$ spins flipped (for free boundary conditions). The single flipped spin can be in $L - 2$ locations, the two flipped spins in $L - 3$ locations and so on. Thus $N_2 = [1 + 2 + 3 + \cdots + (L - 2)] = (L - 2)(L - 1)/2$. The cure for this is to turn on a conjugate field that classifies states both by their energy and number of spins flipped. Now all states with more than one spin flipped do not contribute to N_2 and we get $N_2 = L - 2$. After computing intensive quantities, the field is turned off (set to zero).

Coming back to the spin glass, we note that with a conjugate field, A_i is given by a series

$$A_i = \sum_k A_{ik} v^k , \quad v = e^{-h} , \qquad (1.10)$$

and the free-energy series of Eq. (1.7) becomes

$$F = F_0 + A_{21} u^2 v + A_{22} u^2 v^2 + A_{41} u^4 v + \cdots . \quad (1.11)$$

It is easy to see that the coefficients A_{ik} vanish for odd i.

The next issue is that of finite-size effects. Here again, it is useful to consider the case of the simple Ising model with $J_{ij} = 1$. In this case, finite-size effects arise from lines of excited spins that are affected by the presence of the boundary. For a given lattice size and type (periodic, helical, fixed boundary, etc.), it is straightforward to decide at what order finite-size corrections will contaminate the series since all that is required is to determine the length of shortest path that feels the boundary. One can also determine in a quantitative way how increasing the size of the lattice will improve the order of the expansion.

In the spin-glass case, the situation is not so simple. This is because there is no direct correlation between number of spins flipped and the energy of the state except with respect to a given vacuum. Because of this, there is no systematic way to decide which of the coefficients A_i are "correct" and which are contaminated by finite-size effects. Moreover, there is no way to decide how the situation improves as the volume increases since we cannot compare the vacuum states between different volumes. The only possible resolution we see is an empirical one. We adopt the procedure of determining the series from lattices of progressively increasing sizes and using appropriate extrapolation to get the values of the A's in the thermodynamic limit.

II. A CONCRETE EXAMPLE ON $D = 2$ HELICAL LATTICES

We derive series on generalized helical lattices in $D = 2$. Our lattice is defined as follows: Consider V points along a circle. Neighboring points along the circle are considered to be nearest neighbors in the x direction. Points separated by $r > 1$ steps are considered to be

TABLE I. List of lattices used together with the number of sampled bond configurations.

Volume	r	Effective square lattice linear size	Number of sampled bond configurations
5	3	3	all
6	4	3	all
7	5	3	all
8	3	4	all
9	7	3	all
10	4	4	all
11	4	4	all
12	5	4	15 000
13	5	5	5 000
14	10	5	3 000
15	11	5	3 000
16	10	5	3 000
17	5	5	3 000
18	7	6	3 000
20	6	4	1 829

nearest neighbors in the y direction. We call such a lattice a V/r lattice. Such lattices[5] have been used to generate low-temperature expansions for Ising and Potts models.[6] They have the feature that they minimize finite-size corrections from closed loops. For example, the lattice with $V = 8$ and $r = 3$ (i.e., an 8/3 lattice) is "equivalent" to a periodic lattice of size 4×4 in the sense that the shortest path closed due to finiteness of the lattice is of length $n = 4$.

For each value of V, we chose r so as to maximize the length of the shortest loop closed due to finite-size effects. The lattices we used are listed in Table I. Up to $V = 11$, we generated all bond configurations and so our results are exact. For $V > 11$, we randomly sampled a large number of bond configurations. The number sampled is shown in Table I.
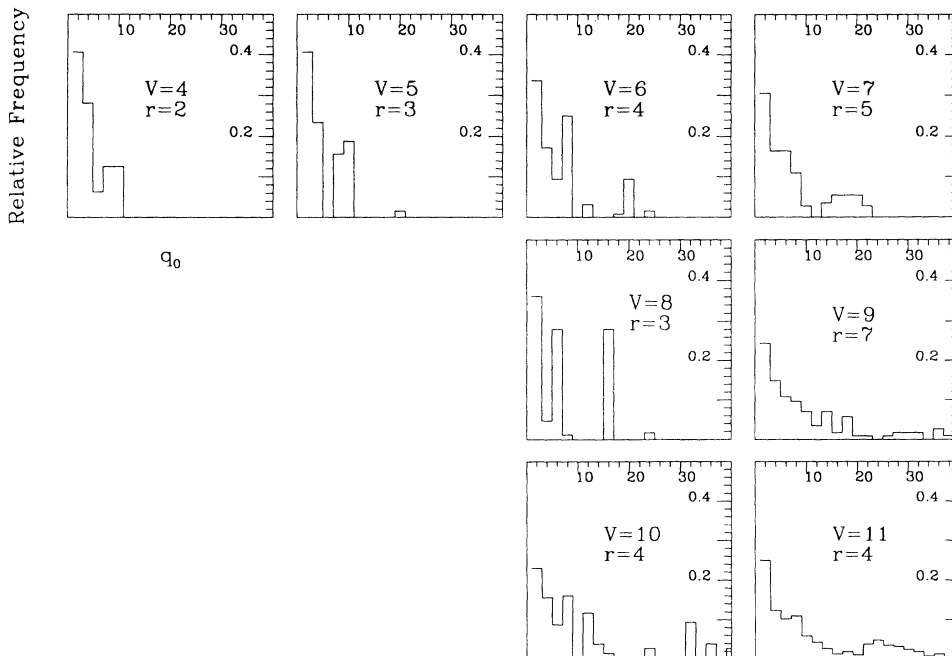

FIG. 1. The distribution of the number of ground states q_0 for $V = 4$ to $V = 11$ over all bond configurations.
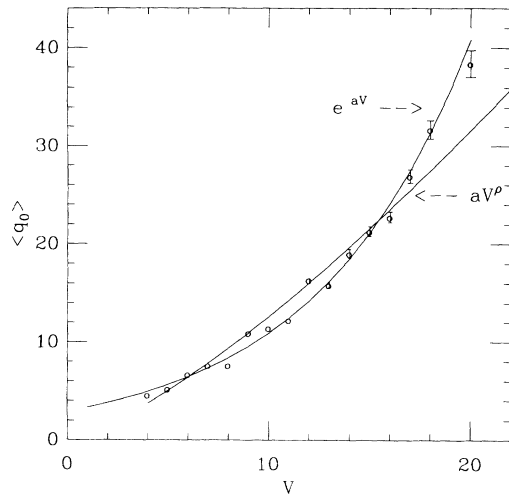
FIG. 2. The average number of ground states $\langle q_0 \rangle$ as a function of volume. The curves are fits to $\langle q_0 \rangle \sim V^\rho$ and $\langle q_0 \rangle \sim \exp(aV)$.

FIG. 4. The free-energy coefficient A_{21} as a function of $1/V$. The thermodynamic value given was obtained by a fit to the plus points.

To gain some insight, we start with a study of ground states as a function of the bond configurations. Figure 1 shows the distribution of the number $q_0(V)$ of ground states for all bond configurations for each V. As is evident from the figure, the distribution spreads to larger values of q_0 as $V \to \infty$. However, for the volumes we considered, the distribution is almost flat and no particular value is selected. In Fig. 2 we plot the average value $\langle q_0 \rangle$ over these distributions for various volumes with fits to an exponential and a power law in V. Our data prefer $\langle q_0 \rangle$ growing like an exponential in V.

We also obtained the distribution of the distances $d(\sigma_0, \sigma_0')$ between pairs of ground states. This was done by computing d for all distinct pairs of vacua for all bond configurations. In Fig. 3 we show the distribution of the bit distance between ground states for $V=20$. The data for other volumes are similar. The symmetry of the figure around $V/2$ is a trivial consequence of the fact that if the configuration σ_0 is a vacuum then so is the
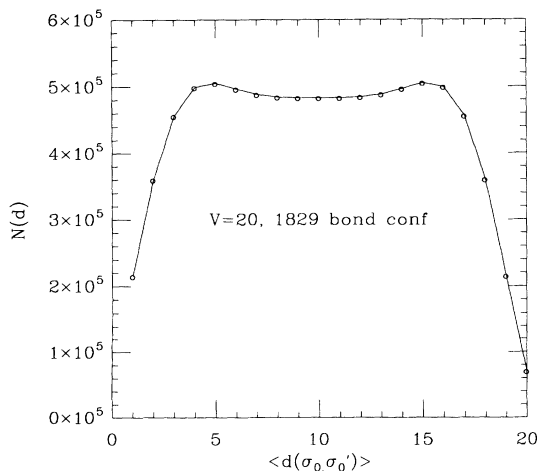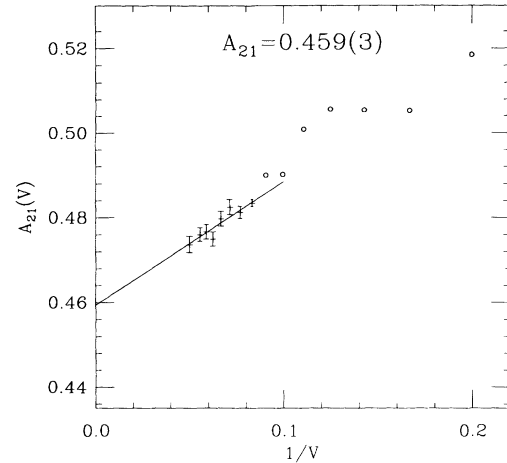
configuration with all spins flipped relative to σ_0. Figure 3 shows that, in contrast to the simple Ising model, in the spin-glass case there are almost equal numbers of vacua separated by all distances from 1 to $V/2$. This is the reason why it is important to carefully define the separation of the states with respect to both the energy and the relative energy as we do here.

Figure 4 shows the coefficient A_{21} as a function of inverse volume $1/V$. The open circles are from averaging over all bond configurations. The pluses are from sampling a finite number of random bond configurations as listed in Table I. Finite-size effects seem nicely parametrized by a $1/V$ dependence and we list the thermodynamic value of A_{21} in this figure by making a linear fit to the data. In Fig. 5 we plot the standard deviation σ_{21} of the A_{21} values as a function of $1/V$. This is to be intrepreted as the "width" of the distribution of A_{21} over all bond configurations. The open circles and pluses have the same interpretation as in Fig. 4 and a linear extrapolation again seems to give an excellent fit. Note that the word "standard deviation" should not suggest that we

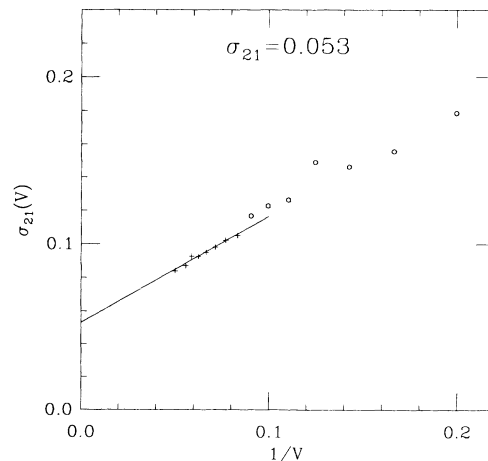FIG. 3. The distribution of bit distances between ground states for $V=20$.

FIG. 5. The standard deviations for the coefficients A_{21} as a function of $1/V$. The thermodynamic value given was obtained by a fit to the plus points.

are estimating a "statistical or systematic error" in our measurement. It represents the *intrinsic* uncertainty in the coefficients due to the fact that they are drawn from a nontrivial distribution. The fact that the thermodynamic value of σ_{21} is nonzero is highly significant. It means that the thermodynamic distribution of A_{21} is nontrivial (*not* a δ function). We interpret this to mean that there is an *inherent* uncertainty in Green's functions in spin glasses, arising from the bond averaging.

We also investigated some other coefficients (A_{22} and A_{41}) and find qualitatively similar results for them. We estimate [see Eq. (1.11)],

$$A_{21} = 0.459(3) , \quad A_{22} = 0.239(5) , \quad A_{41} = 0.479(3) .$$

$$(2.1)$$

The widths of the distributions of these quantities in the thermodynamic limit are $\sigma_{21} = 0.053$, $\sigma_{22} = 0.050$, and $\sigma_{41} = 0.036$, respectively.

III. CONCLUDING REMARKS

We have described a procedure to determine the low-temperature expansion for the free energy of Ising-like spin glasses. We explain why one is forced to do a double expansion in $u = e^{-\beta}$ and $v = e^{-h}$. From numerical calculations on volumes of up to 20 sites, we extract the thermodynamic values for several coefficients of the expansion. We also showed that these coefficients are not simple numbers but rather averages over a nontrivial distribution. This may be the reason why laboratory experiments on spin glasses have a difficult time determining thermodynamic averages.

The concept of self-averaging is based on the nonrigorous idea that a very large system can be divided into a set of smaller (but still macroscopic) systems and self-averaging will follow. This argument only works if the boundary effects are small. As we have emphasized, the number of vacuum states increases exponentially as the system size grows and consequently, the free-energy series coefficients are highly sensitive to the boundary. For this reason, our coefficients have no *a priori* reason to be self-averaging. Another way of saying this is that theoretical proofs of self-averaging generally ignore broken ergodicity and so average over all macrostates, whereas the low-temperature series considered here explicitly takes broken ergodicity into account.

However, note that the free energy can be self-averaging without the coefficients of the low-temperature expansion having the same property. This is because coefficients can be distributions even if the sum of the series is a number (recall that the δ function obtains from a sum over plane waves). The sum of an infinite set of distributions can easily be a number (after proper normalization). For this reason, the fact that the coefficients of the free energy are distributions does not, by itself, prove or disprove the conjecture that the free energy is a number. Our results, based on a few terms in the series, cannot say anything conclusive about self-averaging. One would need many terms in the series to decide this issue.

Finally, the issue of whether or not it is possible to derive series which are long enough to be useful is still open.

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