

This is the accepted manuscript made available via CHORUS. The article has been published as:

# Efficient generation of series expansions for $\pm J$ Ising spin glasses in a classical or a quantum field

R. R. P. Singh and A. P. Young

Phys. Rev. B **96**, 214210 — Published 29 December 2017

DOI: [10.1103/PhysRevB.96.214210](https://doi.org/10.1103/PhysRevB.96.214210)

# Efficient generation of series expansions for $\pm J$ Ising spin-glasses in a classical or a quantum (transverse) field

R. R. P. Singh

*Physics Department, University of California Davis, CA 95616, USA*

A. P. Young

*Physics Department, University of California Santa Cruz, CA 95064, USA*

(Dated: October 30, 2017)

We discuss generation of series expansions for Ising spin-glasses with a symmetric  $\pm J$  (i.e. bimodal) distribution on  $d$ -dimensional hypercubic lattices using linked-cluster methods. Simplifications for the bimodal distribution allow us to go to higher order than for a general distribution. We discuss two types of problem, one classical and one quantum. The classical problem is that of the Ising spin glass in a longitudinal magnetic field,  $h$ , for which we obtain high temperature series expansions in variables  $\tanh(J/T)$  and  $\tanh(h/T)$ . The quantum problem is a  $T = 0$  study of the Ising spin glass in a transverse magnetic field  $h_T$  for which we obtain a perturbation theory in powers of  $J/h_T$ . These methods require (i) enumeration and counting of *all* connected clusters that can be embedded in the lattice up to some order  $n$ , and (ii) an evaluation of the contribution of each cluster for the quantity being calculated, known as the weight. We discuss a general method that takes the much smaller list (and count) of all no free-end (NFE) clusters on a lattice up to some order  $n$ , and automatically generates all other clusters and their counts up to the same order. The weights for finite clusters in both cases have a simple graphical interpretation that allows us to proceed efficiently for a general configuration of the  $\pm J$  bonds, and at the end perform suitable disorder averaging. The order of our computations is limited by the weight calculations for the high-temperature expansions of the classical model, while they are limited by graph counting for the  $T = 0$  quantum system. Details of the calculational methods are presented.

## I. INTRODUCTION

The controlled study of short-range Ising spin-glass models on finite dimensional lattices is well known to be a challenging task [1–3]. Important problems include the question of the de Almeida Thouless instability in a magnetic field [4], and the quantum critical behavior and Griffiths-McCoy singularities in the presence of a transverse quantum field at  $T = 0$  [5–10]. For both these problems it is of great interest to investigate the behavior as a function of dimension.

One of the most successful methods for studying spin glasses is Monte Carlo simulations [3]. Advances in simulation methods have led to substantial insights especially when the dimensionality is not too high. Here we consider an alternative approach, series expansions. Whereas it is difficult to study spin glasses in high dimensions, because the range of (linear) sizes which can be studied is too limited to perform a satisfactory finite-size scaling, the complexity of the series method depends only weakly on dimensionality [11–14], so it is particularly useful for the study of spin glasses in high dimensions. Another advantage of series expansions is that the average over disorder is done exactly. The purpose of this work is to describe an efficient method for calculating such series expansions.

We have recently used these methods to study Ising spin-glasses in classical and quantum (transverse) fields. Series analysis was particularly well behaved for the study of quantum system at  $T = 0$  [15], where we were able to study the interplay of critical and Griffiths-McCoy

singularities as a function of dimensionality and make connections with mean-field theories in high dimensions [16–18] and quantum Monte Carlo simulations in  $d = 2$  and  $d = 3$  [19, 20]. Our results were completely new for higher dimensions and we found the surprising result that the mean-field behavior appeared to persist below the putative upper critical dimension of 8 and down to the known upper critical dimension of the classical system, which is  $d = 6$ . While the convergence for the classical model at finite temperatures, was not as good, we were able to show [21] evidence for de Almeida-Thouless [AT] line of singularities in dimensions 6 and above.

The methods we discuss here are general enough that a class of random classical and quantum problems can be studied using them. Most directly, they can be used to study random ferromagnetic or antiferromagnetic Ising models in a magnetic field. They can also be used to study random Ising models on geometrically frustrated lattices. Certain aspects of our study, will be useful for random Potts, Heisenberg and other models. The graph counting methods are useful for both random and non-random models.

## II. THE LINKED CLUSTER METHOD FOR SERIES EXPANSIONS

### A. The basic idea

Our common framework for developing series expansions for both classical and quantum systems is the

Linked Cluster method [22, 23]. In this method, we consider an extensive property of interest  $P$  and compute  $\lim_{N \rightarrow \infty} P/N$ , where  $N$  is the number of sites of the lattice, i.e. the property  $P$  *per site* in the thermodynamic limit. We expand this quantity in powers of a suitable expansion variable  $x$ . The essence of the Linked Cluster methods is to express  $P/N$  as [22, 23]

$$P/N = \sum_c L(c) \times W(c), \quad (1)$$

where the sum is over all distinct *connected* clusters that can be embedded in the lattice. The quantity  $L(c)$  is called the lattice constant of the cluster  $c$ . It is the number of ways the cluster  $c$  can be embedded in the lattice *per lattice site*. The quantity  $W(c)$  is called the weight of the cluster  $c$  and is given by the recursive relation

$$W(c) = P(c) - \sum_{s \subset c} W(s), \quad (2)$$

where  $P(c)$  is the value of property  $P$  evaluated for cluster  $c$  [24], and the sum over  $s$  is over all “proper” sub-clusters of the cluster  $c$  (i.e. the sum excludes  $c$  itself). Thus a series calculation requires:

1. enumeration and counting of all relevant clusters, and
2. calculation of the weight of each cluster, which needs to be expanded as a power series in the expansion variable  $x$ .

The weight of a cluster with  $n$  bonds can be shown to be of order [22, 23]  $x^n$ . Thus, summing up contributions from all clusters with  $n$  or fewer bonds gives the series expansion for  $P/N$  to order  $n$ .

For certain problems such as classical spin-glasses in zero-field, many quantities only require a limited type of clusters. One of the most efficient such method is a star-graph expansion [12, 25] that requires only clusters that do not have articulation points. An articulation point is a node which, if removed, would split the graph into disconnected pieces. Certain other calculations [11, 14, 22] may only require clusters with zero or at most two free ends (a free end is a site with only one other site connected to it). Figure 1 shows several clusters with no free ends (NFE). Clearly all star graphs, except the trivial one with one bond, are of the NFE type, whereas some NFE graphs are not stars, an example being cluster (b) in Fig. 1. However, the problems we study here with classical and quantum fields require consideration of *all* connected clusters. Since this part of the calculation is common to both classical and quantum study we discuss this enumeration and counting problem first. We then separately consider the weight calculations for the quantum and classical systems.

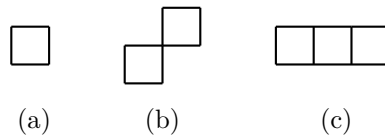


FIG. 1: Three examples of graphs with no free ends. Of these, (a) and (c) are also star graphs, but (b) is not because it can be cut in two by removing the vertex where the two squares join.

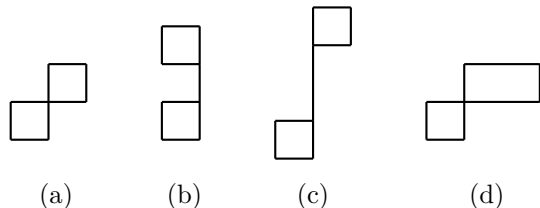


FIG. 2: A complete list of non-star NFE graphs (a) through (d) that can be embedded in hypercubic lattices with 10 or fewer bonds.

## B. Graph enumeration and lattice constants

We consider nearest-neighbor models on  $d$ -dimensional hypercubic lattices. Furthermore, we will only consider properties such as spin-glass susceptibility where the weights of a cluster only depend on the connectivity (or adjacency matrix) of the cluster and not on the many ways in which the cluster may be embedded in the  $d$ -dimensional lattice. Hence we will not be able to calculate, for example, the correlation length which requires a knowledge of the vector between each pair of sites in the cluster. In this section we will use the terms cluster and graph interchangeably to mean the same thing.

Following Fisher and Gaunt [26], the lattice constant for such a cluster  $c$  in dimension  $d$  can be expressed as

$$L_d(c) = \sum_{m=m_{min}}^{m_{max}} \binom{d}{m} l_m(c), \quad (3)$$

where  $\binom{d}{m}$  is the binomial coefficient. Here  $l_m(c)$  is the count of those embeddings of the cluster  $c$  that extend in  $m$  dimensions. The limits of the summation  $m_{min}$  and  $m_{max}$  refer to the minimum and maximum dimension in which the cluster embeddings can extend. Clearly a cluster with  $n$  bonds can not extend in more than  $d = n$  dimensions, but if there are closed loops then  $m_{max}$  is less than  $n$ . Using Eq. (3), one can go back and forth between  $L_d(c)$  and  $l_m(c)$ . One first calculates  $L_d(c)$  in different dimensions up to the maximum dimension where there is an embedding of cluster  $c$  and then uses Eq. (3) to obtain  $l_m(c)$ . Once that is done, one can now readily obtain the lattice constants in arbitrary dimension by using Eq. (3) again. For the rest of this section we will assume that we are working with a fixed dimensionality  $d$ .

TABLE I: Counts of embeddings  $l_m(c)$  of the non-star, NFE clusters in Fig. 2 that extend in exactly  $m$  dimensions. Note that none of these NFE clusters extend beyond 6 dimensions.

cluster in Fig. 2	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$
(a)	2	24	48	0	0
(b)	8	168	576	480	0
(c)	20	792	5184	10080	5760
(d)	8	552	3168	3840	0

We will now describe a method to obtain all connected clusters up to order 10 in any dimension starting from the NFE clusters and their lattice constants. The lattice constants of star-graphs to order 11 in general dimension were provided by Ditzian and Kadanoff [25]. According to their Table III, there are only 17 star-graphs with 10 or less bonds. In addition, there are 4 non-star, NFE graphs up to order 10, and these are shown in Figure 2 while their lattice constants are given in Table I. Hence the number of NFE graphs up to order 10 is 21. By contrast, we find that the *total* number of graphs with 10 or less bonds increases to 933 when free-ends are allowed. Furthermore, general graphs with 10-bonds can be embedded in all dimensions up to  $d = 10$ , and their lattice constants can become enormous. To get an idea, up to 10 bonds the largest lattice constant for an NFE graph for  $d \leq 10$  is about  $10^7$ . By contrast, lattice constant for graphs with free ends can be of order  $10^{13}$  for  $d \leq 10$ . Thus a *direct* enumeration of all embeddings of general graphs becomes very challenging especially in high dimensions.

Instead, we will develop here a method which generates a list of all graphs (including those with free ends) and their lattice constants from the lattice constants of graphs with no free-ends, without any further *explicit* enumeration of the embeddings.

It is evident from the meaning of a free-end that any graph with  $n + 1$  bonds that has at least one free-end can be obtained from some graph with  $n$  bonds by attaching a bond to one of its sites. Such an  $n$ -bond graph can be obtained by just cutting off the last bond on one of the free-ends.

To generate the lattice constants of these free-end graphs, we will use a method along the lines of early work of Domb [27, 28] and Fisher and Gaunt [26]. These authors showed that there are relationships between lattice constants of different graphs. For example, if we take a chain of length  $n$  and attach to it an additional bond at the end, it will create a chain of length  $n + 1$ . Thus the lattice constant for a chain of length  $n + 1$  should be related to the lattice constant for a chain of length  $n$  times the number of ways a bond can be added to the ends, except that upon addition of the bond, it can touch one of the existing sites of the chain thus forming either a closed loop of length  $n + 1$  or a tadpole graph [26, 27], see Fig. 3.

For concreteness consider  $n = 7$ . Let us call the length

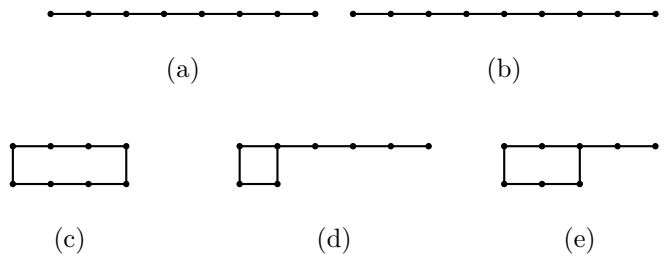


FIG. 3: Various graphs arising in Eq. (4): (a) linear graph of length 7 denoted  $c_7$ , (b) linear graph of length 8 denoted  $c_8$ , (c) polygon of length 8 denoted  $p_8$ , (d) tadpole graph with one free-end denoted  $t_{4,4}$ , (e) tadpole graph with one free-end denoted  $t_{6,2}$ .

7 chain as  $c_7$ , length 8 chain as  $c_8$ , the polygon of length 8 as  $p_8$ , a tadpole with a length 2 chain attached to a loop of length 6 as  $t_{6,2}$ , and a tadpole with a length 4 chain attached to a loop of length 4 as  $t_{4,4}$ . These graphs are shown in Fig. 3. On a  $d$ -dimensional lattice there are  $2d - 1$  ways to add a bond at either end of a chain. Hence, the relationship is:

$$2(2d - 1)L_d(c_7) = 2L_d(c_8) + 2 \times 8L_d(p_8) + 2L_d(t_{6,2}) + 2L_d(t_{4,4}), \quad (4)$$

where the factors in front of the lattice constants are related to the symmetries of the graphs. The factor of 2 on the left hand side is related to the fact that the bond can be added on either end. The factor of 2 before  $L_d(c_8)$  is because the same embedding of  $c_8$  can arise in two ways by addition of last bond on left or right. The factor of  $2 \times 8$  for  $l_d(p_8)$  is because any one of the 8 bonds of the polygon could have been added to a chain to form the polygon and it could be added from either end. The factor of 2 for the other two graphs is because the last bond added that forms the tadpole from a chain of length 7 must be one of the two bonds inside the loop next to the site with valency 3. Such relations exist whenever a bond is added to a graph.

Before we discuss our method further, we need to define a graph theoretic property called the cyclomatic number. The cyclomatic number of a graph is defined by the number of independent cycles in the graph [28]. It equals  $n - m + 1$ , where  $n$  is number of bonds and  $m$  is number of sites. Thus a tree graph, which has one less bond than sites, has a cyclomatic number of 0 in agreement with there being no cycles. The important thing to note about the above Eq. (4) is that only one graph on the right hand side, the first one, has the same cyclomatic number as the graph on the left hand side. All other graphs have one higher cyclomatic number as an additional loop has been formed. Thus, if the lattice constants of all graphs with higher cyclomatic number are already known, this equation can help us determine  $L_d(c_8)$  from  $L_d(c_7)$ .

We will use the facts that (i) all graphs with free-ends

can be obtained by adding a bond to some other graph with one less bond, (ii) lattice constants of graphs can be related by some relation such as in Eq. (4), and (iii) highest cyclomatic number graphs in any order must either have no free-ends or can be obtained by adding a bond to a smaller no free-end graph with the same cyclomatic number, without the creation of any additional graphs on the right hand side of Eq. (4). Using these facts, and working in order of decreasing cyclomatic number, we next describe an algorithm that allows us to obtain a list of all graphs and their lattice constants.

We work in order of increasing number of bonds, and, for a given number of bonds, we work in order of decreasing cyclomatic number. Suppose a complete list of all graphs in order  $n$  is already available. Then, we obtain the complete list of all graphs in order  $n + 1$  by adding bonds to all  $n$  bond graphs in all possible ways, plus the additional NFE graphs of order  $n + 1$ , whose counts already exist. Note that in such a scheme the same graph can be generated many times and the duplicates have to be removed using standard methods [22, 23]. Then the only thing that remains is find the analog of Eq. (4) every time a new graph is found. We do this by an automated computer algorithm discussed next. This automated algorithm for recognizing the desired equation from which lattice constant of the new graph can be read off is one of the most important developments in this paper.

Consider a parent graph  $g_p$  with  $n$  bonds and  $m$  sites. We generate a daughter graph  $g_d$  with  $n + 1$  bonds and  $m + 1$  sites, either with an extra free end or with the length of one of the free ends extended by one (see Fig. 4), by (a) picking a site  $i$  of the parent graph and (b) adding a bond connecting this site to an additional site, which we label as  $m + 1$ .

We would like to find an equation that relates the lattice constant of the daughter graph to the lattice constant of the parent graph. In order to have such a relation, we need to know what other graphs can result in the process of adding a bond from site  $i$  to one of the existing sites of the graph. We can find a list of all such graphs by attempting to add a bond between site  $i$  and any other site of the graph and see if that forms an allowed graph with one additional loop. Let us remember that when graphs are generated in order of decreasing cyclomatic number (decreasing number of loops) then counts for such graphs will already be known. Let us say we obtain  $q$  such graphs we can label 1 through  $q$  and let the valency of the site  $i$  in the parent graph be  $v$ . Then the desired equation is

$$L_d(g_d) = \frac{(2d - v)s_p L_d(g_p) - \sum_{n=1}^q s_n L_d(g_n)}{s_d} \quad (5)$$

Here,  $s_p$  is the number of equivalent sites in the parent graph where addition of a bond also leads to same daughter graph,  $s_d$  is the number of ways the daughter graph can be generated from the parent graph and  $s_n$  is the number of ways the graph  $g_n$  gets generated by adding a bond from a site of the parent graph equivalent to  $i$  to an

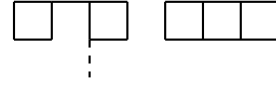


FIG. 4: Example of a parent graph,  $g_p$  (on the left without the dashed line), a daughter graph,  $g_d$ , on the left with the dashed line added, and additional graph  $g_1$  (on the right) needed to get a closed equation for the lattice constants.

other site. All these factors  $v$ ,  $s_d$ ,  $s_p$  and  $s_n$  depend only on the connectivity or adjacency matrix of the graph and not its actual embeddings in a particular lattice. Hence, they can be calculated by an automated computer algorithm from the adjacency matrix of the graph. Thus, the lattice constant of the graph  $g_d$  can be obtained.

We have already seen one example of such a relation in Fig. 3 and Eq. (4). Another example is shown in Fig. 4. The parent graph is a 9-bond, 8-site graph with no free ends. Adding a bond as shown in the figure as a protruding dashed line, produces a 10-bond, 9-site daughter graph with one free end. In this case  $v = 2$ ,  $s_p = 4$  and  $s_d = 1$ . There is only one other type of graph that can result by connecting the site under consideration to one of the existing sites in the parent graph. That is a 10-bond 8-site graph also shown in Fig. 4. In this problem  $s_n = 4$  as there are two bonds whose removal can lead to the parent graph from the daughter graph and at either end of the bond the site becomes equivalent to our addition site in the parent graph. So, the equation becomes

$$L_d(g_d) = 4(2d - 2)L_d(g_p) - 4L_d(g_1) \quad (6)$$

When this procedure is followed starting with a single-bond graph and its count, which is  $d$ , together with a list of all NFE graphs, a complete list and count of all graphs results.

For the Sherrington-Kirkpatrick [2] model, every spin interacts with every other spin and the variance of the interactions is proportional to  $1/N$  to get a sensible thermodynamic limit. In our work we obtain this model by taking the limit  $d \rightarrow \infty$  and scaling the variance of the interactions by  $1/(2d)$  (the inverse of the number of neighbors). It is well known that only tree graphs are needed in this limit. Since NFE graphs all have at least one closed loop, their counts become negligible together with those of all graphs with at least one loop, relative to the tree graphs. The relevant count of these tree graphs is simply given by the largest power of  $d$  that arises in Eq. (3). To obtain a list and count of just the tree graphs, one can start with a single bond graph and carry out the procedure discussed above ignoring any graphs with loops. In that case, equations such as Eq. (5) have only the parent and daughter graph and no additional graphs. One can show that, the factors of  $s_d$  and  $s_p$  in the Eq. (5) lead to a count of these tree graphs with  $n$ -bonds that



can be expressed as

$$L_{SK}(c) = \frac{(2d)^n}{p_c}, \quad (7)$$

where  $p_c$  is the symmetry factor of the graph, defined by the number of permutations of the sites of the graph that leaves the graph invariant. The factor of  $(2d)^n$  then cancels with the  $n$  factors of the variance of the bonds, leading to a result which is independent of  $d$  for  $d \rightarrow \infty$ .

We have generated graphs to 14th order for SK model, to 10th order for general  $d$  and also to 14th order in  $d = 2$  and  $d = 3$ , where NFE graph counts had been previously generated by an explicit enumeration [29]. Thus, graph counting is currently limited by the availability of counts of NFE graphs.

### III. FINITE CLUSTER CALCULATIONS FOR QUANTUM ISING SPIN GLASSES

#### A. Some Preliminaries

For the transverse field Ising spin glass calculations, the unperturbed Hamiltonian is the transverse field so we work in a representation in which this is diagonal, rather than the usual representation in which the Ising spin glass part is diagonal. The Hamiltonian is therefore

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1 \quad (8)$$

where the unperturbed Hamiltonian is

$$\mathcal{H}_0 = - \sum_k \sigma_k^z, \quad (9)$$

in which we have set the transverse field,  $h^T$ , equal to 1, and the perturbation is the Ising spin glass part,

$$\mathcal{H}_1 = \sum_{\langle j,k \rangle} J_{jk} \sigma_j^x \sigma_k^x. \quad (10)$$

In this section we consider a single cluster with  $N$  sites and  $B$  bonds. The interactions take values

$$J_b = \epsilon_b J, \text{ with } \epsilon_b = \pm 1, \quad (11)$$

where  $(b = 1, 2, \dots, B)$ . Averages over disorder are simple with this bimodal distribution since

$$J_b^n = \begin{cases} J^n, & (n \text{ even}), \\ \epsilon_b J^n, & (n \text{ odd}), \end{cases} \quad (12)$$

Hence, in addition to the *overall* order of a term in the series, we only need to keep track of the *parity* of the number of times each *individual* bond is used. And, at the end the disorder average for  $J_b^n$  is simply  $J^n$  for  $n$  even and zero for  $n$  odd.

We write  $\mathcal{H}_1$  as

$$\mathcal{H}_1 = J \sum_{b=1}^B \tilde{\mathcal{H}}_b \quad (13)$$

where

$$\tilde{\mathcal{H}}_b = \epsilon_b \sigma_{b_1}^x \sigma_{b_2}^x \quad (14)$$

is the perturbation due to bond  $b$ , which has the effect of flipping the two spins,  $b_1$  and  $b_2$ , connected to it, i.e.

$$\text{flip}_b(S_{b_1}, S_{b_2}) = (-S_{b_1}, -S_{b_2}) \quad (15)$$

where the notation  $\text{flip}_b$  means act with bond  $b$  to flip the two spins connected to it, and  $S_{b_1}$  etc. refers to the value of  $\sigma_{b_1}^x$  in the basis state being considered.

We note that the perturbation has no diagonal matrix elements among the basis states and, in particular,  $\langle 0 | \tilde{\mathcal{H}}_b | 0 \rangle = 0$ .

We will develop perturbation theory for the ground state of the cluster in powers of the  $J_b$ . The unperturbed ground state,  $|0\rangle$ , has all spins along  $z$  and has energy  $E_0$ . We denote a general unperturbed eigenstate by  $|\alpha\rangle$  and its energy by  $E_\alpha$ . These will be our (normalized) basis states.

The perturbation expansion is in powers of  $J$ , but we also need to specify *which* bonds have been used. Acting with a bond flips both spins attached to this bond, see Eq. (15), so acting twice with the bond leaves the original state unchanged. The result of acting on the ground state with a product of bond terms can therefore be specified by a set of bits,  $l_i$ , which give the *parity* of the number of times bond  $i$  has acted:  $l_i = 0$  for an even number of times, and  $l_i = 1$  for an odd number. Similarly, since the bonds take only the two values  $\pm J$ , see Eq. (11), a product of  $n$  bonds, some of which might occur more than once, can also be written in terms of the  $l_i$  as

$$\prod_k J_k = J^n \left( \prod_{b=1}^B \epsilon_b^{l_b} \right), \quad (16)$$

where we recall that  $B$  is the number of bonds in the cluster.) To make the notation more compact we write the bits  $\{l_b\}$  as a single integer  $L (= 0, 1, \dots, 2^B - 1)$  where

$$L = \sum_{b=1}^B 2^{b-1} l_b. \quad (17)$$

In other words,  $l_b$  is the  $b$ -th bit in the bitwise representation of  $L$ . The unperturbed ground state  $|0\rangle$  has  $L = 0$ .

Acting with a set of bonds specified by an integer  $L$  on

$|0\rangle$  gives a basis state  $|\alpha\rangle$  as follows:

$$|\alpha\rangle = \prod_b (\sigma_{b_1}^x \sigma_{b_2}^x)^{l_b^L} |0\rangle, \quad (18)$$

where  $l_b^L$  is the parity of the number of times (1, odd or 0, even) of the number of times the  $b$ -th bond appears in the graph represented by  $L$ . Hence a given value of  $L$  *uniquely* specifies a state. However, the same  $|\alpha\rangle$  can be obtained in different ways by flipping different sets of bonds, so the mapping is *many to one*.

As an example, for a set of bonds which form closed loops each spin is flipped an even number of times so it maps to the ground state, as does acting with no bonds,  $L = 0$ . We denote the set of bond strings which map to  $|0\rangle$  by  $\{L_0\}$ . A general bond string  $L$  which maps to a basis state  $|\alpha\rangle$  is written as

$$L = L_0 \oplus \alpha \quad (19)$$

where  $\oplus$  means bitwise addition modulo 2. For  $L_0 = 0$  we have  $\alpha = L$  so, in this scheme, we label a spin state by *one representative string* of bonds  $L$  which maps to that state. We emphasize that we are representing a basis state by one of the sets of *bonds* that maps to it from  $|0\rangle$  (flipping both spins of the bond), rather than by the *spins themselves*.

One way to choose values of  $\alpha$  and  $L_0$  for a given bond string integer  $L$  is to run through consecutive integers starting from 0 up to  $2^B - 1$ . For each integer one determines the spin configuration. If it has not previously occurred then we choose this  $L$  to be the representative value for the spin state, i.e. this bond state is specified by  $\alpha = L$  and  $L_0 = 0$ . If the spin state has been met before we associate  $L$  with two integers, the value of  $\alpha$  of that (previously obtained) spin state, and  $L_0$  where  $L = L_0 \oplus \alpha$ . In this way, we determine necessary lookup tables  $\alpha(L)$  and  $L_0(L)$ . For an example see Appendix A, especially Table II.

We have already said that there  $2^B$  values of  $L$  which specify the different bond strings. Since each bond flips two spins, only states in the even subspace (i.e. those with an even number of spins flipped) will be generated from the unperturbed ground state. Hence the number of spin states generated will be half their total number, i.e.  $2^{N-1}$ . Consequently, the number of values of the bond strings  $L_0$  which map to the ground state (and which also gives the number of times *each* spin state is generated from all possible bond strings), is the ratio  $2^B/2^{N-1} = 2^{B+1-N}$ . Note that this is  $2^{C_n}$  where  $C_n$  is the cyclomatic number discussed in Sec. IIB, i.e. the number of independent cycles in the graph.

We will also need information about the result of acting with an *additional* bond  $b$  on an existing bond string. If the original bond string is represented by an integer  $L$  then adding one more bond  $b$  gives an integer  $L'$  where

$$L' = \text{flip}_b L, \quad (20)$$

i.e.  $L'$  is trivially obtained from  $L$  by flipping the  $b$ -th bit of  $L$ . Now  $L = L_0 \oplus \alpha$ , and if  $L' = L'_0 \oplus \alpha'$  we need to compute  $\alpha'$  and  $L'_0$  from

$$(\alpha', L'_0) = \text{flip}_b (\alpha, L_0), \quad (21)$$

for each  $(\alpha, L_0)$  and  $b$ . The precise mapping will depend on the (arbitrary) choice of which of the possible  $L$ 's which map to state  $|\alpha\rangle$  is taken to be the “representative” value (i.e. the one which goes with  $L_0 = 0$ ). Given  $L_0$  and  $\alpha$  one first determines  $L$  from  $L = L_0 \oplus \alpha$ , then gets  $L'$  from  $L' = \text{flip}_B L$ , and finally uses the lookup tables,  $\alpha' = \alpha(L')$ ,  $L'_0 = L_0(L')$  to get  $\alpha'$  and  $L'_0$ .

## B. Series for the ground state energy and wavefunction

We now set up the perturbation expansions for the ground state energy and ground state wave function. The ground state wave function  $|\psi_g\rangle$  will mix into the unperturbed ground state  $|0\rangle$  other basis states  $|\alpha\rangle$  as follows,

$$|\psi_g\rangle = |0\rangle + \sum_{n=1}^{\infty} J^n \sum_{L_0, \alpha \neq 0} C_n^{\alpha \oplus L_0} G^{\alpha \oplus L_0} |\alpha\rangle, \quad (22)$$

where

$$G^{\alpha \oplus L_0} = \left( \prod_{b=1}^B \epsilon_b^{l_b^{\alpha \oplus L_0}} \right) \quad (23)$$

is a graph represented by an integer  $L = \alpha \oplus L_0$  with  $b$  bits, where  $l_b^{\alpha \oplus L_0} = 1$  if the  $b$ -th interaction  $\epsilon_b$  appears an odd number of times and 0 if it appears an even number of times. Graphically, an edge  $b$  is present in the graph  $G$  if the interaction  $\epsilon_b$  appears an odd number of times, otherwise it is absent.

To get the ground state energy, we start with the unperturbed ground state and act with perturbations which must lead, at the end, back to the unperturbed ground state. Hence the only perturbations which contribute to the ground state are those in the set  $\{L_0\}$ , i.e.

$$E_g = E_0 + \sum_{n=1}^{\infty} J^n \sum_{L_0} e_n^{L_0} G^{L_0}. \quad (24)$$

We are free to choose the normalization of the ground state and do so by requiring that the coefficient of the unperturbed ground state  $|0\rangle$  in Eq. (22) is precisely unity, so  $|0\rangle$  is excluded from the sum over states  $|\alpha\rangle$  in Eq. (22). Expectation values therefore have to be calculated from

$$\langle \dots \rangle = \frac{\langle \psi_g | \dots | \psi_g \rangle}{\langle \psi_g | \psi_g \rangle}, \quad (25)$$

where the normalizing denominator is given by

$$\langle \psi_g | \psi_g \rangle = 1 + \sum_{n=1}^{\infty} J^n \sum_{m=0}^n \sum_{\alpha} \sum_{L_0, L'_0} C_m^{\alpha \oplus L_0} C_{n-m}^{\alpha \oplus L'_0} G^{L''_0}, \quad (26)$$

in which  $L''_0 = L_0 \oplus L'_0$ . This series can be written

$$\langle \psi_g | \psi_g \rangle = 1 + \sum_{n=1} J^n \sum_{L_0} U(n, L_0) G^{L_0}, \quad (27)$$

where we recall that the graph  $G^{L_0}$  indicates which bonds have been used to generate the term, and

$$U(n, L_0) = \sum_{m=0}^n \sum_{\alpha} \sum_{L'_0} C_m^{\alpha \oplus L'_0} C_{n-m}^{\alpha \oplus L'_0 \oplus L_0}. \quad (28)$$

It is necessary to keep track of which bonds have been used in order to the final average over disorder. Note

that in this expression we only have to sum over bond configurations  $L_0$  which map the ground state back to the ground state.

The numerator in Eq. (25) can also be written in a form similar to Eq. (27) except that we are no longer restricted to bond configurations which map the ground state to itself, so

$$\langle \psi_g | \cdots | \psi_g \rangle = \sum_{n=0} J^n \sum_{L=0}^{2^B-1} V(n, L) G^L, \quad (29)$$

where the coefficients  $V(n, L)$  can be determined from the ground state expansion coefficients  $C_n^{\alpha \oplus L_0}$  and a knowledge of the matrix elements of the operator  $(\cdots)$ . We discuss in Appendix B how to divide the series in Eq. (29) by that in (27) efficiently.

The Schrödinger equation is

---


$$\left\{ \mathcal{H}_0 + J \sum_{b=1}^B \tilde{\mathcal{H}}_b \right\} \left\{ |0\rangle + \sum_{n=1}^{\infty} J^n \sum_{L_0, \alpha \neq 0} C_n^{\alpha \oplus L_0} G^{\alpha \oplus L_0} |\alpha\rangle \right\} = \left\{ E_0 + \sum_{n=1}^{\infty} J^n \sum_{L_0} e_n^{L_0} G^{L_0} \right\} \left\{ |0\rangle + \sum_{n=1}^{\infty} J^n \sum_{L_0, \alpha \neq 0} C_n^{\alpha \oplus L_0} G^{\alpha \oplus L_0} |\alpha\rangle \right\}. \quad (30)$$


---

To proceed we first multiply both sides of Eq. (30) on the left by  $\langle 0|$  and equate the terms with the same order  $n$  and bond graph  $G^{\alpha \oplus L_0}$  on both sides. For  $n = 0$  this trivially gives  $\langle 0 | \mathcal{H}_0 | 0 \rangle = E_0 \langle 0 | 0 \rangle$ . For  $n > 0$  we have

$$\sum_{b=1}^B C_{n-1}^{\alpha \oplus L'_0} \langle 0 | \sigma_{b_1}^x \sigma_{b_2}^x | \alpha \rangle = e_n^{L_0}, \quad (31)$$

where

$$(\alpha, L'_0) = \text{flip}_b(0, L_0). \quad (32)$$

The matrix element is one so we have

$$e_n^{L_0} = \sum_{b=1}^B C_{n-1}^{\alpha \oplus L'_0}. \quad (33)$$

Next we multiply both sides of Eq. (30) on the left by

$\langle \gamma |$  where  $\gamma \neq 0$ . This gives

$$(E_0 - E_\gamma) C_n^{\gamma \oplus L_0} = \sum_{b=1}^B \langle \gamma | \sigma_{b_1}^x \sigma_{b_2}^x | \alpha \rangle C_{n-1}^{\alpha \oplus L'_0} - \sum_{m=1}^{n-1} \sum_{L'_0} e_m^{L'_0} C_{n-m}^{\gamma \oplus L_0 \oplus L'_0}, \quad (34)$$

where, in the first term on the RHS,

$$(\alpha, L'_0) = \text{flip}_b(\gamma, L_0). \quad (35)$$

Simplifying we get

$$C_n^{\gamma \oplus L_0} = \frac{1}{E_0 - E_\gamma} \left\{ \sum_{b=1}^B C_{n-1}^{\alpha \oplus L'_0} - \sum_{m=1}^{n-1} \sum_{L'_0} e_m^{L'_0} C_{n-m}^{\gamma \oplus L_0 \oplus L'_0} \right\}, \quad (36)$$

where we again note Eq. (35). In the second term on the RHS of Eq. (36), the terms with  $m = n$  and  $m = 0$  are not included, as can be seen by looking at the RHS of Eq. (30). For the case of  $n = 1$ , the second term on the



RHS of Eq. (36) does not occur, and, in the first term, one has  $\alpha = L_0 = L'_0 = 0$  and  $C_0^0 = 1$ .

To determine the terms in the expansion one proceeds as follows:

1. Use Eq. (36) with  $n = 1$  to determine the first order correction to the wave function.
2. Use Eq. (33) with  $n = 2$  to get the second order contribution to the energy.
3. Use Eq. (36) with  $n = 2$  to determine the second order correction to the wave function.
4. Repeat steps 2 and 3 to go to higher orders.

Note that in the RHS of Eq. (33), and in the first term on the RHS of Eq. (36), for each bond  $b$  only one value of  $\alpha$  and  $L'_0$  will contribute, given by Eqs. (32) and (35) respectively.

In order to do the calculation we need to run through spin states (labeled here by  $\alpha$ ), and bond strings which map to the ground state (labeled here by  $L_0$ ) *consecutively*. We therefore construct appropriate arrays to map from consecutive entries to  $\alpha$  (and to  $L_0$ ), and for the inverse mapping from  $\alpha$  (and  $L_0$ ) to consecutive entries.

Having obtained the wavefunction coefficients in the expansion in Eq. (22), the series for each expectation value of interest is obtained from Eq. (25), in which the numerator and denominator have the forms in Eq. (29) and (27) respectively. An efficient way to divide these series is given in Appendix B.

In a spin glass the series for the expectation value has to be squared, see Appendix B, and then finally averaged over the bond disorder. Since the expectation value of a bond is 0, the only terms which survive after bond averaging are those where each bond appears an even number of times, i.e. those in which the bond string  $L$ , defined in Eq. (17), is zero.

### C. Series for the spin glass susceptibility

Next we want to compute the spin glass susceptibility. This can be done by computing the change in energy to quadratic order in local, magnetic fields which couple to  $\sigma^x$ . Writing

$$E_g(\{h\}) = E_g(0) + \frac{1}{2} \sum_{i,j} \chi_{ij} h_i h_j + O(h^4), \quad (37)$$

the spin glass susceptibility is given by

$$\chi_{SG} = \sum_{i,j} [\chi_{ij}^2]_{av}. \quad (38)$$

We will consider the field to act on just two sites at a time, “ $i$ ” and “ $j$ ”. Hence the Hamiltonian we consider is

$$\mathcal{H} = - \sum_k \sigma_k^z + J \sum_{b=1}^B \epsilon_b \sigma_{b_1}^x \sigma_{b_2}^x + (h_i \sigma_i^x + h_j \sigma_j^x). \quad (39)$$

(Recall that  $b$  is a bond and  $\epsilon_b = \pm 1$ .)

Up to now we have only needed to consider the even spin subspace, that is the unperturbed ground state and all states obtained from it by flipping pairs of spins. Recall from Sec. III B that these can be characterized by an integer  $\alpha$  such that the  $b$ -th bit of  $\alpha$  is 1 if bond  $b$  is used to generate the spin state an odd number of times and zero otherwise, see Eq. (18). Several integers  $L$  (i.e. several sets of bonds) can generate the same spin state  $\alpha$  and the graph  $G$  of bonds is given by Eq. (23).

How do we extend these ideas to the odd subspace? First of all we write a state in the even subspace as  $|\alpha\rangle_e$  and one in the odd subspace as  $|\alpha\rangle_o$ . The unperturbed ground state in the even subspace,  $|0\rangle_e$ , has all spins along the  $+x$  direction. We define the corresponding state in the odd subspace,  $|0\rangle_o$ , to be the state obtained from  $|0\rangle_e$  by flipping one of the spins coupled to one of the fields in Eq. (39), let's say “ $i$ ”, i.e.

$$\sigma_i^x |0\rangle_e = |0\rangle_o, \quad (40)$$

Other states in the odd subspace are then obtained in the same way as those in the even subspace, so

$$\sigma_i^x |\alpha\rangle_e = |\alpha\rangle_o, \quad (41)$$

and similarly  $\sigma_i^x |\alpha\rangle_o = |\alpha\rangle_e$ .

This representation is a convenient way to describe spin states obtained by flipping the spin at site “ $i$ ” due to the field term in Eq. (39) and then acting with pair flips due to the bonds. However, we also will need to describe the spin state obtained by using the field to flip the other site with a field in Eq. (39), namely “ $j$ ”, and then act with a set of pairwise bond flips. To do this we will need the state that has just sites “ $i$ ” and “ $j$ ” flipped. This will be represented by string of bonds between these two sites, which we will call  $\alpha_{ij}$ . Except for tree graphs there will be several bond strings which do this, differing by closed-loop graphs specified by  $L_0$ . We choose the one with  $L_0 = 0$  (the empty graph).

Hence, flipping spin “ $j$ ” and acting with bond graph  $\alpha$  gives

$$\sigma_j^x |\alpha\rangle_e = \left( \prod_{b \in \alpha_{ij}} \sigma_{b_1}^x \sigma_{b_2}^x \right) \sigma_i^x |\alpha\rangle_e = \sigma_i^x |\alpha \oplus \alpha_{ij}\rangle_e = |\alpha \oplus \alpha_{ij}\rangle_o. \quad (42)$$

We will compute the series expansion for the ground state energy and wave function in powers of  $J$  and up to second order in  $h_i$  and  $h_j$ . The ground state energy is an even function of the fields so the new piece is quadratic

in  $h_i$  and  $h_j$ . Each term in the perturbation expansion for the GS energy involves generating excited states from the unperturbed ground state and ending up back in the unperturbed ground state. Hence the quadratic terms in the energy involve one of the following processes: (i) use  $h_i$  to flip spin “ $i$ ” and flip it back, (ii) use  $h_j$  to flip spin

“ $j$ ” and flip it back, (iii) use  $h_i$  to flip spin “ $i$ ” and  $h_j$  to flip spin “ $j$ ”, and then flip both these back with a bond string between them. The ground state wave function will have terms linear in the fields as well as quadratic.

We therefore make the following ansatz.

$$E_g = E_0 + \sum_{n=1}^{\infty} J^n \sum_{L_0} e_n^{L_0} G^{L_0} + \sum_{n=0}^{\infty} J^n \sum_{L_0} \left[ h_i^2 g_n^{(ii),L_0} G^{L_0} + h_j^2 g_n^{(jj),L_0} G^{L_0} + h_i h_j g_n^{(ij),L_0} G^{L_0 \oplus \alpha_{ij}} \right], \quad (43)$$

$$\begin{aligned} |\psi_g\rangle &= |0\rangle_e + \sum_{n=1}^{\infty} J^n \sum_{\alpha \neq 0, L_0} C_n^{\alpha \oplus L_0} G^{\alpha \oplus L_0} |\alpha\rangle_e \\ &+ \sum_{n=0}^{\infty} J^n \sum_{(\text{all } \alpha), L_0} \left( h_i A_n^{(i), \alpha \oplus L_0} G^{\alpha \oplus L_0} |\alpha\rangle_o + h_j A_n^{(j), \alpha \oplus L_0} G^{\alpha \oplus L_0} |\alpha \oplus \alpha_{ij}\rangle_o \right) \\ &+ \sum_{n=0}^{\infty} J^n \sum_{\alpha \neq 0, L_0} \left( h_i^2 D_n^{(ii), \alpha \oplus L_0} G^{\alpha \oplus L_0} + h_j^2 D_n^{(jj), \alpha \oplus L_0} G^{\alpha \oplus L_0} \right) |\alpha\rangle_e \\ &+ \sum_{n=0}^{\infty} J^n \sum_{\alpha \neq \alpha_{ij}, L_0} h_i h_j D_n^{(ij), \alpha \oplus L_0} G^{\alpha \oplus L_0} |\alpha \oplus \alpha_{ij}\rangle_e. \end{aligned} \quad (44)$$

As for the zero field case in Sec. III B we write down the Schrödinger equation with these ansatzes, and project out the terms separately by multiplying on the left by  ${}_e\langle 0|$ ,  ${}_e\langle \alpha|$  (for  $\alpha \neq 0$ ), and  ${}_o\langle \alpha|$ .

After some algebra we find the following results. For order  $n = 0$  (remember  $n$  is the lower index) all quantities are zero except for

$$C_0^0 = 1, \quad A_0^{(i),0} = -\frac{1}{2}, \quad g_0^{(ii),0} = -\frac{1}{2}, \quad D_0^{(ij),0} = \frac{1}{4}. \quad (45)$$

The quantities which are independent of the  $h_i$ , namely  $e_n^{L_0}$  and  $C_n^{\alpha \oplus L_0}$ , have only to be calculated once, and the formulae for them were already obtained in Eqs. (33) and (36) in Sec. III B above.

The quantities involving one field  $h_i$  have to be calculated  $N$  times, once for each value of the site  $i$  where the field is applied. The description of the odd states is set up separately for each value of  $i$ , such that  $|0\rangle_o = \sigma_i^x |0\rangle_e$ . We find

$$g_n^{(ii),L_0} = \sum_{b=1}^B D_{n-1}^{(ii), \alpha \oplus L_0'} + A_n^{(i),L_0}, \quad (46)$$

$$\begin{aligned} A_n^{(i), \alpha \oplus L_0} &= \frac{1}{E_0 - E_{\alpha}^{\text{odd}}} \\ &\left\{ \sum_{b=1}^B A_{n-1}^{(i), \gamma \oplus L_0'} + C_n^{\alpha \oplus L_0} - \sum_{m=1}^n \sum_{L_0'} e_m^{L_0'} A_{n-m}^{(i), \alpha \oplus L_0 \oplus L_0'} \right\}, \end{aligned} \quad (47)$$

$$\begin{aligned} D_n^{(ii), \alpha \oplus L_0} &= \frac{1}{E_0 - E_{\alpha}} \left\{ \sum_{b=1}^B D_{n-1}^{(ii), \gamma \oplus L_0'} + A_n^{(i), \alpha \oplus L_0} \right. \\ &\left. - \sum_{m=0}^{n-1} \sum_{L_0'} g_m^{(ii), L_0'} C_{n-m}^{\alpha \oplus L_0 \oplus L_0'} - \sum_{m=1}^n \sum_{L_0'} e_m^{L_0'} D_{n-m}^{(ii), \alpha \oplus L_0 \oplus L_0'} \right\}. \end{aligned} \quad (48)$$

Next we give expressions for quantities involving two fields  $h_i$  and  $h_j$ . These have to be calculated  $N(N-1)/2$  times, once for each pair  $i$  and  $j$ . The description of the odd states has to be set up separately for each pair. We find

$$g_n^{(ij),L_0} = \sum_{b=1}^B D_{n-1}^{(ij), \alpha \oplus \alpha_{ij} \oplus L_0'} + A_n^{(i), \alpha_{ij} \oplus L_0} + A_n^{(j), \alpha_{ij} \oplus L_0}, \quad (49)$$

$$D_n^{(ij), \alpha \oplus L_0} = \frac{1}{E_0 - E_{\alpha \oplus \alpha_{ij}}} \left\{ \sum_{b=1}^B D_{n-1}^{(ij), \gamma \oplus L'_0} + A_n^{(i), \alpha \oplus L_0} \right. \\ \left. + A_n^{(j), \alpha \oplus L_0} - \sum_{m=0}^{n-1} \sum_{L'_0} g_m^{(ij), L'_0} C_{n-m}^{\alpha \oplus \alpha_{ij} \oplus L_0 \oplus L'_0} \right. \\ \left. - \sum_{m=1}^n \sum_{L'_0} e_m^{L'_0} D_{n-m}^{(ij), \alpha \oplus L_0 \oplus L'_0} \right\}. \quad (50)$$

The procedure to calculate the series iteratively is therefore as follows:

- Compute the zero field quantities first. (Note that  $C_0^0 = 1$ .)
  - Use Eq. (36) with  $n = 1$  to compute the first order correction to the wave function.
  - Use Eq. (33) followed by Eq. (36) with  $n = 2, 3, \dots$  to compute successive orders.

Equation (33) is not applied for  $n = 1$  because the RHS of that equation vanishes in this case.

- Compute quantities involving one field. (Note that  $A_0^{(i), 0} = -1/2, g_0^{(ii), 0} = -1/2$ .) Use Eq. (47) followed by Eq. (48) followed by Eq. (46) iteratively with  $n = 1, 2, 3, \dots$
- Compute quantities involving two fields. (Note that  $D_0^{(ij), 0} = -1/4$ .) Use Eq. (50) followed by Eq. (49) iteratively with  $n = 1, 2, 3, \dots$

Our goal is to calculate the spin glass susceptibility  $\chi_{SG}$  given by Eq. (38). Now the change in energy is related to the local susceptibilities  $\chi_{ij}$  given by Eq. (37). Comparing with Eq. (43) we see that

$$\chi_{ii} = 2 \sum_{n=0}^{\infty} J^n \sum_{L_0} g_n^{(ii), L_0} G^{L_0}, \quad (51)$$

$$\chi_{ij} = \sum_{n=0}^{\infty} J^n \sum_{L_0} g_n^{(ij), L_0} G^{L_0 \oplus \alpha_{ij}}, \quad (i \neq j), \quad (52)$$

$$\chi_{ji} = \chi_{ij}. \quad (53)$$

We square these expressions, and then average over disorder which gives except for the graph with no bonds,  $G^0$ , because the average of each bond,  $J\epsilon_b$ , is zero. Hence

$$[\chi_{ii}^2]_{\text{av}} = 4 \sum_{n=0}^{\infty} J^n \sum_{L_0} \sum_{m=0}^n g_m^{(ii), L_0} g_{n-m}^{(ii), L_0}, \quad (54)$$

$$[\chi_{ij}^2]_{\text{av}} = \sum_{n=0}^{\infty} J^n \sum_{L_0} \sum_{m=0}^n g_m^{(ij), L_0} g_{n-m}^{(ij), L_0}, \quad (i \neq j). \quad (55)$$

Summing these expression over sites gives  $\chi_{SG}$  according to Eq. (38).

#### IV. FINITE CLUSTER CALCULATIONS FOR ISING SPIN-GLASSES IN A CLASSICAL FIELD

In this section, we consider weight calculations for the Ising spin-glass in a classical field. The problem is defined by the Hamiltonian:

$$\mathcal{H} = - \sum_{\langle i, j \rangle} J_{ij} S_i S_j - h \sum_{i=1}^N S_i, \quad (56)$$

where the  $S_i$  are Ising spins which take values  $\pm 1$ , and the interactions  $J_{ij}$  are *quenched* random variables, again with a bimodal distribution,  $J_{ij} = \pm J$  with equal probability.

The key quantity of interest is the spin glass susceptibility  $\chi_{SG}$  where

$$\chi_{SG} = \frac{1}{N} \sum_{i, j=1}^N \left[ \left( \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle \right)^2 \right]_{\text{av}}. \quad (57)$$

For a fixed value of  $h$  we expand the susceptibility in powers of

$$w = \tanh^2(J/T). \quad (58)$$

The coefficient of  $w^n$  turns out to be a polynomial of order  $2n + 2$  in

$$u = \tanh^2(h/T), \quad (59)$$

so

$$\chi_{SG}(w, u) = \sum_{n=0}^{\infty} \left( \sum_{m=0}^{2n+2} a_{n,m} u^m \right) w^n. \quad (60)$$

Our goal is to calculate the series coefficients for the spin-glass susceptibility on a *finite* cluster with  $B$  bonds and  $N$  sites.

We begin with the partition function

$$Z \equiv \text{Tr} \exp(-\beta H) \\ = \sum_{\{S_i = \pm 1\}} \exp \left( \beta \sum_{\langle i, j \rangle} J_{ij} S_i S_j + \beta h \sum_i S_i \right). \quad (61)$$

We use the relations

$$\exp(\beta J_{ij} S_i S_j) = \cosh \beta J (1 + v_{ij} S_i S_j), \quad (62)$$

with  $v_{ij} = \tanh \beta J_{ij}$ , and

$$\exp(\beta h S_i) = \cosh \beta h (1 + r S_i), \quad (63)$$

with  $r = \tanh \beta h$ . Let us define

$$Z' = \frac{Z}{(\cosh \beta J)^B (2 \cosh \beta h)^N}, \quad (64)$$

where, as stated above,  $B$  is the number of bonds and  $N$  the number of sites in the cluster. Then,

$$Z' = \frac{\text{Tr} \prod_{\langle i,j \rangle} (1 + v_{ij} S_i S_j) \prod_i (1 + r S_i)}{2^N}. \quad (65)$$

The main task is to expand  $Z'$  in powers of the  $v_{ij}$  and  $r$ . When the two products are expanded the trace will be non-zero only if each spin occurs an even number of times. In that case the trace will give a factor of  $2^N$ , canceling that factor in the denominator. The first product over the bonds has  $2^B$  terms and each one combines uniquely with a suitable number of powers of  $r$  from the second term to give a non-zero contribution. Thus the trace results in precisely  $2^B$  terms. Thermal averages such as  $\langle S_i S_j \rangle$  or  $\langle S_i \rangle$  can be expressed as a ratio of two such traces each of which has  $2^B$  terms.

These terms have a simple graphical representation. To illustrate that, we consider an elementary square graph consisting of 4 sites and 4 bonds shown in Fig. 5. The expressions for the numerator of  $\langle S_a S_d \rangle$  and  $\langle S_a \rangle$  and their common denominator are shown graphically in Figs. 6–8. A line on bond  $j$  gives a factor of  $\tanh(\beta J_j)$ , and we have defined

$$r = \tanh(\beta h). \quad (66)$$

Note that in zero field there would have been only two non-zero terms for the graphs in Figs. 6 and 7 (and non at all in Fig. 8), but now 16 terms contribute for all these graphs. This is one of the main sources of complexity in working with a non-zero field.

The explicit expressions for the graphs in Figs. 6–8 are as follows. Labeling the bonds as in Fig. 5, and noting that  $v_i \equiv \tanh \beta J_i = \epsilon_i \tanh \beta J = \epsilon_i v$  where

$$v = \tanh(\beta J) \quad (67)$$

and  $\epsilon_i = \pm 1$ , the expression for  $Z'$  in Fig. 6 is

$$\begin{aligned} Z' = & 1 + v^4 \epsilon_1 \epsilon_2 \epsilon_3 \epsilon_4 + r^4 v^2 (\epsilon_2 \epsilon_4 + \epsilon_1 \epsilon_3) + \\ & r^2 v (\epsilon_4 + \epsilon_2 + \epsilon_1 + \epsilon_3) + \\ & r^2 v^2 (\epsilon_4 \epsilon_1 + \epsilon_1 \epsilon_2 + \epsilon_2 \epsilon_3 + \epsilon_3 \epsilon_4) + \\ & r^2 v^3 (\epsilon_1 \epsilon_3 \epsilon_4 + \epsilon_1 \epsilon_2 \epsilon_3 + \epsilon_1 \epsilon_2 \epsilon_4 + \epsilon_2 \epsilon_3 \epsilon_4). \end{aligned} \quad (68)$$

Similarly in Fig. 7, the expression for  $Z' \langle S_a S_d \rangle$  is

$$\begin{aligned} Z' \langle S_a S_d \rangle = & v \epsilon_4 + v^3 \epsilon_1 \epsilon_2 \epsilon_3 + r^4 (v^3 \epsilon_1 \epsilon_3 \epsilon_4 + v \epsilon_2) + \\ & r^2 (1 + v^4 \epsilon_1 \epsilon_2 \epsilon_3 \epsilon_4) + r^2 v (\epsilon_1 + \epsilon_3) + \\ & r^2 v^2 (\epsilon_4 \epsilon_1 + \epsilon_1 \epsilon_2 + \epsilon_2 \epsilon_3 + \epsilon_3 \epsilon_4 + \epsilon_2 \epsilon_4 + \epsilon_1 \epsilon_3) + \\ & r^2 v^3 (\epsilon_1 \epsilon_2 \epsilon_4 + \epsilon_2 \epsilon_3 \epsilon_4). \end{aligned} \quad (69)$$

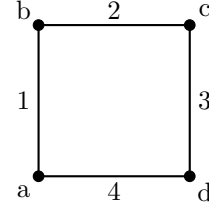


FIG. 5: Labeling of spins a, b, c and d (at the corners) and bonds (1, 2, 3, and 4) on the edges, for the example in Appendix A

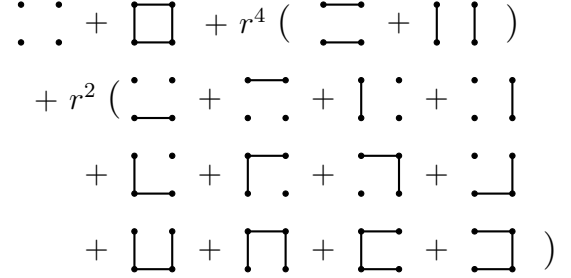


FIG. 6: Expansion of  $Z'$  for the square graph in Fig. 5 in which  $r = \tanh(\beta h)$ . A line on bond  $j$  gives a factor of  $\tanh(\beta J_j) = \epsilon_j \tanh(\beta J) = \epsilon_j v$ . Each point with an odd number of lines going to it has a factor of  $r$ . Note that only the first two terms contribute in zero field.

Finally the expression for  $Z' \langle S_a \rangle$  in Fig. 8 is

$$\begin{aligned} Z' \langle S_a \rangle = & r + r v^4 (1 + \epsilon_1 \epsilon_2 \epsilon_3 \epsilon_4) + r v (\epsilon_1 + \epsilon_4) + \\ & r v^2 (\epsilon_3 \epsilon_4 + \epsilon_1 \epsilon_2) + r v^3 (\epsilon_1 \epsilon_2 \epsilon_3 + \epsilon_2 \epsilon_3 \epsilon_4) + \\ & r^3 v (\epsilon_2 + \epsilon_3) + r^3 v^2 (\epsilon_4 \epsilon_1 + \epsilon_2 \epsilon_3 + \epsilon_2 \epsilon_4 + \epsilon_1 \epsilon_3) + \\ & r^3 v^3 (\epsilon_4 \epsilon_1 \epsilon_2 + \epsilon_1 \epsilon_3 \epsilon_4). \end{aligned} \quad (70)$$

The products of the  $\epsilon_i$  are visualized as a bond graph  $G^L$ , as discussed in Sec. III B and illustrated in Appendix A for the square cluster in Fig. 5. The series can be divided and multiplied as discussed in Appendix B, the only difference here being that we have a double series in  $v = \tanh(\beta J)$  and  $r = \tanh(\beta h)$ , but the methods of Appendix B are easily generalized to this case.

## V. CONCLUSIONS

In this manuscript, we have discussed a linked cluster based method for calculating series expansions for Ising spin-glasses in a classical (longitudinal) field and a quantum (transverse) field. These expansions require *all* connected clusters (which we also denote by graphs) that can be embedded on the lattice. The calculations require the counting and enumeration of such graphs on the lattice, along with the weight calculations for the quantities being computed, which are expanded as series expansions for each graph.

$$\begin{aligned}
& \cdot \cdot + \text{---} + r^4 ( \text{---} + \text{---} ) \\
& + r^2 ( \cdot \cdot + \text{---} + \text{---} + \text{---} \\
& + \text{---} + \text{---} + \text{---} + \text{---} \\
& + \text{---} + \text{---} + \text{---} + \text{---} )
\end{aligned}$$

FIG. 7: Expansion of  $Z'\langle S_a S_d \rangle$  for the square graph in Fig. 5(a) in which  $r = \tanh(\beta h)$ . The two spins  $S_a$  and  $S_d$  are on the lower horizontal bond of the square and are indicated by the larger circles. There is a factor of  $r$  for each small circle which has an odd number of lines going to it, and also a factor of  $r$  for each large circle with an even number of lines going to it. Note again that only the first two terms contribute in zero field.

$$\begin{aligned}
& r ( \cdot \cdot + \text{---} + \text{---} + \text{---} \\
& + \text{---} + \text{---} + \text{---} + \text{---} ) \\
& + r^3 ( \text{---} + \text{---} + \text{---} + \text{---} \\
& + \text{---} + \text{---} + \text{---} + \text{---} )
\end{aligned}$$

FIG. 8: Expansion of  $Z'\langle S_a \rangle$  for the square graph in Fig. 5 in which  $r = \tanh(\beta h)$ . The spin  $S_a$  is the lower left spin, indicated by the larger circle. There is a factor of  $r$  for each small circle which has an odd number of lines going to it, and also a factor of  $r$  for each large circle with an even number of lines going to it. Note that  $Z'\langle S_a \rangle$  is odd in the field and so vanishes identically in zero field.

We have discussed a method that takes a small list of graphs with no free ends and obtains a complete list of all graphs by using the computer to automatically generate suitable relations between lattice constants of graphs with a free-end added to an existing graph thus avoiding the need for an explicit enumeration of all lattice embeddings. Using available counts for no free-end graphs in  $d = 2$  and  $d = 3$  we have generated all graphs in these cases to 14-th order. In higher than  $3d$ , we have only generated these counts to 10-th order using previously available star-graph counts. In future, it should be possible to extend these counts in higher dimensions to at least 14-th order using the results of Brooks-Harris, Aharony and collaborators [14, 30].

We have discussed weight calculations for classical and quantum cases. The  $\pm J$  model provides great simplification in these calculations since we only need to keep track of the odd-even-ness of each bond before the final disorder averaging, see Eq. (12). This allows for a simple graphical representation of the expansion that can be efficiently dealt with on the computer. We find that

the weight calculations for the transverse-field case at  $T = 0$  are particularly efficient so that the calculations are primarily limited by our ability to generate counts for no free-end graphs. Thus, it should be possible to extend the series especially in dimensionality greater than or equal to four when such graph counts are available. By contrast, the finite temperature weight calculations for classical spin-glasses in a field are much more time consuming, and it would be difficult to extend these series to much higher orders using the present methods.

We have recently used these methods to study Ising spin-glasses in classical and quantum (transverse) fields. Series analysis was particularly well behaved for the study of quantum system at  $T = 0$  [15], where we were able to study the interplay of critical and Griffiths-McCoy singularities as a function of dimensionality. While the convergence for the classical model at finite temperatures, was not as good, we were able to show [21] evidence for de Almeida-Thouless [AT] line of singularities in dimensions 6 and above.

These methods are general enough that a class of random classical and quantum models can be studied using them. Most straight-forwardly, they can be used to study random-bond ferromagnets or antiferromagnets in a magnetic field. They can also be used to study random Ising models in a field on geometrically frustrated lattices. Certain aspects of our study, will be useful for random Potts, Heisenberg and other models as well. Our graph counting methods are useful for both random and non-random lattice models, where study of high-dimensionality may be important.

### Acknowledgments

One of us (APY) would like to thank the hospitality of the Indian Institute of Science, Bangalore and the support of a DST-IISc Centenary Chair Professorship. He is particularly grateful for stimulating discussions with H. Krishnamurthy which initiated this project. The work of RRPS is supported in part by US NSF grant number DMR-1306048.

### Appendix A: An example of labeling states

We illustrate the method of labeling states by considering the example of a single square shown in Fig. 5. We label the bonds by 1, 2, 3 and 4, and the spins by a, b, c and d. The ground state has all spins up,  $|\uparrow\uparrow\uparrow\uparrow\rangle$ .

The sequence in the spin labeling is a, b, c and d from right to left, so, for example, the state with spin c flipped is  $|\uparrow\downarrow\uparrow\uparrow\rangle$ . Bond 1 is between spins a and b, bond 2 between spins b and c etc. We represent the graph of bonds which are used to generate the spin states by an integer  $L$ , where each bit of  $L$  corresponds to a bond, and is 1 if that bond is used to flip the two spins attached to it and 0 otherwise. The bits of  $L$  are bonds 4, 3, 2 and 1



TABLE II: Labeling of states for the graph consisting of a single square shown in Fig. 5. Note that in this graph, which has a single cycle, each spin state is generated in two ways by acting with bonds. Increasing  $L$  from 0, we label the state by  $\alpha = L$  and  $L_0 = 0$  as long as the state has not been found before. If the state has been found before we associate this bond integer  $L$  with the same value of  $\alpha$  as found before but now  $L_0 = 15$  (which corresponds to the single closed loop of bonds for this graph). In all cases one has  $L = \alpha \oplus L_0$  where  $\oplus$  is bitwise addition modulo 2. Columns four and five of this table give us, for this graph, the lookup tables  $\alpha(L)$  and  $L_0(L)$  which are needed in the computations. In this way we can relate a set of bonds, specified by an integer  $L$  to the label  $\alpha$  for the spin state obtained by acting with those bonds on the unperturbed ground state. We also need to store the spin configuration for each value of  $\alpha$  (column three).

$L$	bits of $L$	spin state	$\alpha$	$L_0$
0	0000	$ \uparrow\uparrow\uparrow\uparrow\rangle$	0	0
1	0001	$ \uparrow\uparrow\uparrow\downarrow\rangle$	1	0
2	0010	$ \uparrow\uparrow\downarrow\uparrow\rangle$	2	0
3	0011	$ \uparrow\uparrow\downarrow\downarrow\rangle$	3	0
4	0100	$ \uparrow\downarrow\uparrow\uparrow\rangle$	4	0
5	0101	$ \uparrow\downarrow\uparrow\downarrow\rangle$	5	0
6	0110	$ \uparrow\downarrow\downarrow\uparrow\rangle$	6	0
7	0111	$ \uparrow\downarrow\downarrow\downarrow\rangle$	7	0
8	1000	$ \downarrow\uparrow\uparrow\uparrow\rangle$	7	15
9	1001	$ \downarrow\uparrow\uparrow\downarrow\rangle$	6	15
10	1010	$ \downarrow\uparrow\downarrow\uparrow\rangle$	5	15
11	1011	$ \downarrow\uparrow\downarrow\downarrow\rangle$	4	15
12	1100	$ \downarrow\downarrow\uparrow\uparrow\rangle$	3	15
13	1101	$ \downarrow\downarrow\uparrow\downarrow\rangle$	2	15
14	1110	$ \downarrow\downarrow\downarrow\uparrow\rangle$	1	15
15	1111	$ \downarrow\downarrow\downarrow\downarrow\rangle$	0	15

from left to right. Hence acting with bond 3, which has bit representation  $L = 0100$ , i.e.  $L = 4$ , flips spins c and d and so gives state  $|\downarrow\downarrow\uparrow\uparrow\rangle$ .

In this example, which has a single loop, each spin state can be generated by two bond graphs. For example, the ground state is represented by the two bond integers  $L = 0$  and 15 with bit representations  $L = 0000$  and  $L = 1111$ . The lookup tables  $\alpha(L)$  and  $L_0(L)$ , needed in the computations, are shown in columns four and five of Table II, and are obtained as described in the figure caption. The spin configurations for each  $\alpha$ , also needed in the computations, are shown in column three.

## Appendix B: Dividing Series

Suppose we have two series of a single variable  $x$ ,  $f(x) = \sum_{n=0}^{\infty} a_n x^n$  and  $g(x) = \sum_{n=0}^{\infty} b_n x^n$  and we want

the ratio,  $h(x) = \sum_{n=0}^{\infty} c_n x^n$ , i.e.

$$\sum_{n=0}^{\infty} c_n x^n = \frac{\sum_{n=0}^{\infty} a_n x^n}{\sum_{n=0}^{\infty} b_n x^n}. \quad (\text{B1})$$

We are given the  $a_n$  and  $b_n$  and want the  $c_n$ . We assume without loss of generality that  $b_0 = 1$ . The simplest way to compute the ratio in Eq. (B1) is to multiply both sides by the denominator of the RHS, i.e.

$$\left(\sum_{n=0}^{\infty} b_n x^n\right) \left(\sum_{n=0}^{\infty} c_n x^n\right) = \sum_{n=0}^{\infty} a_n x^n. \quad (\text{B2})$$

Equating coefficients of powers of  $x$  on both sides one obtains the recursive equation

$$c_n = a_n - \sum_{k=1}^n b_k c_{n-k} \quad (n > 0), \quad (\text{B3})$$

with  $c_0 = a_0$ . Using Eq. (B3) for  $n = 1, 2, 3, \dots$  in order, determines the coefficients  $c_n$ .

In the present case, the series have an extra parameter, the integer  $L$  representing the bonds that were used to generate this term, see Eqs. (25), (29) and (27). In other words we have to generalize the above to

$$\begin{aligned} f(x) &= \sum_{n=0}^{\infty} \sum_{L=0}^{2^B-1} a_{n,L} x^n, \\ g(x) &= \sum_{n=0}^{\infty} \sum_{L=0}^{2^B-1} b_{n,L} x^n, \\ h(x) \equiv f(x)/g(x) &= \sum_{n=0}^{\infty} \sum_{L=0}^{2^B-1} c_{n,L} x^n, \end{aligned} \quad (\text{B4})$$

where  $b_{0,0} = 1$  and  $b_{0,L} = L$  for  $L \neq 0$ . Proceeding as before, and noting that the factors of  $L$  are combined using bitwise addition modulo 2, we have

$$c_{n,L} = a_{n,L} - \sum_{k=1}^n \sum_{L'=0}^{2^B-1} b_{k,L'} c_{n-k,L' \oplus L}. \quad (\text{B5})$$

We also have to multiply series which is easily done by the above methods. The final stage is to square the correlation functions and average over disorder, which means that only the resulting term with  $L = 0$  survives.

[1] S. F. Edwards and P. W. Anderson, *Theory of spin glasses*, J. Phys. F **5**, 965 (1975).

[2] D. Sherrington and S. Kirkpatrick, *Solvable model of a spin glass*, Phys. Rev. Lett. **35**, 1792 (1975).

- [3] K. Binder and A. P. Young, *Spin glasses: Experimental facts, theoretical concepts and open questions*, Rev. Mod. Phys. **58**, 801 (1986).
- [4] J. R. L. de Almeida and D. J. Thouless, *Stability of the Sherrington-Kirkpatrick solution of a spin glass model*, J. Phys. A **11**, 983 (1978).
- [5] D. S. Fisher, *Random transverse field Ising spin chains*, Phys. Rev. Lett. **69**, 534 (1992).
- [6] D. S. Fisher, *Critical behavior of random transverse-field Ising spin chains*, Phys. Rev. B **51**, 6411 (1995).
- [7] R. B. Griffiths, *Nonanalytic behavior above the critical point in a random Ising ferromagnet*, Phys. Rev. Lett. **23**, 17 (1969).
- [8] B. M. McCoy, *Incompleteness of the critical exponent description for ferromagnetic systems containing random impurities*, Phys. Rev. Lett. **23**, 383 (1969).
- [9] B. M. McCoy, *Theory of a two-dimensional Ising model with random impurities. III. boundary effects*, Phys. Rev. **188**, 1014 (1969).
- [10] T. Vojta, *Quantum Griffiths effects and smeared phase transitions in metals: theory and experiment*, J. Low Temp. Phys. **161**, 299 (2010).
- [11] R. Fisch and A. B. Harris, *Series study of a spin-glass model in continuous dimensionality*, Phys. Rev. Lett. **38**, 785 (1977).
- [12] R. R. P. Singh and S. Chakravarty, *Critical behavior of an Ising spin-glass*, Phys. Rev. Lett. **57**, 245 (1986).
- [13] M. E. Fisher and R. R. P. Singh, *Critical points, large-dimensionality expansions, and the Ising spin-glass*, in *Disorder in Physical Systems*, edited by G. Grimmett and D. J. A. Welsh (Oxford University Press, Oxford, 1990).
- [14] L. Klein, J. Adler, A. Aharony, A. B. Harris, and Y. Meir, *Series expansions for the Ising spin glass in general dimension*, Phys. Rev. B **43**, 11249 (1991).
- [15] R. R. P. Singh and A. P. Young, *Critical and Griffiths-McCoy singularities in quantum Ising spin-glasses on  $d$ -dimensional hypercubic lattices: A series expansion study* (2017), (arXiv:1707.01557).
- [16] J. Ye, S. Sachdev, and N. Read, *Solvable spin glass of quantum rotors*, Phys. Rev. Lett. **70**, 4011 (1993).
- [17] D. A. Huse and J. Miller, *Zero-temperature critical behavior of the infinite-range quantum Ising spin glass*, Phys. Rev. Lett. **70**, 3147 (1993).
- [18] N. Read, S. Sachdev, and J. Ye, *Landau theory of quantum spin glasses of rotors and Ising spins*, Phys. Rev. B **52**, 384 (1995).
- [19] H. Rieger and A. P. Young, *Zero temperature quantum phase transition of a two-dimensional Ising spin glass*, Phys. Rev. Lett. **72**, 4141 (1994).
- [20] M. Guo, R. N. Bhatt, and D. A. Huse, *Quantum critical behavior of a three-dimensional Ising spin glass in a transverse magnetic field*, Phys. Rev. Lett. **72**, 4137 (1994).
- [21] R. R. P. Singh and A. P. Young, *On the Almeida-Thouless instability in short-range Ising spin-glasses*, Phys. Rev. E **96**, 012127 (2017), (arXiv:1705.01164).
- [22] J. Oitmaa, C. Hamer, and W. Zheng, *Series Expansion Methods for strongly interacting lattice models* (Cambridge University, Cambridge, 2006).
- [23] M. P. Gelfand, R. R. P. Singh, and D. Huse, *Perturbation expansions for quantum many-body systems*, J. Stat. Phys. **59**, 1093 (1990).
- [24] Note that the since the lattice constant is the number of embeddings *per site*, our calculation gives the intensive quantity  $P/N$  even though  $P(c)$  is the *total* value of  $P$  for cluster  $c$ .
- [25] R. V. Ditzian and L. P. Kadanoff, *High-temperature expansion methods for Ising systems with quenched impurities*, Phys. Rev. B **19**, 4631 (1979).
- [26] M. E. Fisher and D. S. Gaunt, *Ising model and self-avoiding walks on hypercubic lattices and “high-density” expansions*, Phys. Rev. **133**, A224 (1964).
- [27] C. Domb, *On the theory of cooperative phenomena in crystals*, Adv. Phys. **9**, 149 (1960).
- [28] C. Domb, *Graph theory and embeddings*, in *Phase Transitions and Critical Phenomena*, Vol. 3, edited by C. Domb and M. Green (Academic Press, London, 1973), p. 1.
- [29] T. Devakul, N. Sherman, and R. R. P. Singh, unpublished data.
- [30] D. Daboul, I. Chang, and A. Aharony, *Test of universality in the Ising spin glass using high temperature graph expansion*, Physics of Condensed Matter **41**, 231 (2004), arXiv:cond-mat/0408167.