Partition Function Zeros of an Ising Spin Glass

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Abstract

We study the pattern of zeros emerging from exact partition function evaluations of Ising spin glasses on conventional finite lattices of varying sizes. A large number of random bond configurations are probed in the framework of quenched averages. This study is motivated by the relationship between hierarchical lattice models whose partition function zeros fall on Julia sets and chaotic renormalization group flows in such models with frustration, and by the possible connection of the latter with spin glass behaviour. In any finite volume, the simultaneous distribution of the zeros of all partition functions can be viewed as part of the more general problem of finding the location of all the zeros of a certain class of random polynomials with positive integer coefficients. Some aspects of this problem have been studied in various areas of mathematics, and we show in particular how polynomial mappings which are used in graph theory to classify graphs, may help in characterizing the distribution of zeros. We finally discuss the possible limiting set of these zeros as the volume is sent to infinity.

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1 Introduction

The $\pm K$ Ising spin glass is defined as a nearest-neighbour Ising model with the bonds $K_{ij}$ (between sites $i$ and $j$) distributed randomly on the lattice according to a given probability distribution. The nature of the possible phase transitions of such a model in different number of dimensions is, despite its apparently simple structure, still to a large extent an open question (see, e.g., ref. [1] for some excellent recent reviews). But also the physics of the ordered or disordered spin glass phases themselves needs to be better understood. Although models of the Ising spin glass kind are easy to define formally, finding even approximate analytic solutions is strikingly difficult. And just as the highly complex dynamics of these models makes it hard to apply conventional analytical approaches, this very aspect is also making standard Monte Carlo simulations almost prohibitively difficult for systems of sufficiently large volume [2]. The combination of both analytical and numerical problems when studying these models thus seems to call for a new approach, one that combines the exactness of analytical treatments with the computational power of numerical evaluations. One very interesting combined approach of this kind is the exact evaluation of finite-volume spin glass partition functions [3, 4], based on either variations of the numerical transfer-matrix method or, specific to two dimensions, exact rewrites of the full high-temperature expansion. With exact (numerical, but with as high precision as needed, without statistical or systematic errors) computation of Ising spin glass partition functions the apparently only remaining problem in “solving” the theory is to understand how the results scale as the finite volumes are taken to infinity.

The purpose of the present paper is to discuss the distribution of partition-function zeros of a $\pm K$ Ising spin glass with nearest neighbour interaction in the complex temperature plane. This is a problem for which the method of exact finite-volume partition function evaluation is the only one applicable, and we will use it as the basis of our analysis. With present-day numerical routines, the location of the partition-function zeros can be found to any practically required precision for systems of very large volumes. In this location of the partition-function zeros is hidden a wealth of information about the model under study. This has been known since the study of Ising model zeros in both the complex activity plane [5] (the so-called Lee-Yang zeros), and, more relevant for the present discussion, the complex temperature plane [6] (now known as Fisher zeros). Of particular interest are of course those partition-function zeros that lie close to possible phase transition points or phase transition boundaries for physical, real, values of the magnetic field or temperature. Here renormalization group (RG) considerations or finite-size scaling theory give direct connections to universal critical properties of the system [4, 8]. But, as we will argue below, at least for the case of Ising spin glasses, the location of partition function zeros away from critical points may also provide non-trivial information about the dynamics of the system.

Our original motivation for the present study was precisely to use the overall location of partition function zeros to shed new light on the nature of spin glass interactions at arbitrary points in the phase diagram as, for example, real-space renormalization group transformations are taking us to the long-distance limit. This approach was inspired in an indirect way by the very interesting suggestion of McKay, Berker and Kirkpatrick [9] that an exactly solvable “frustrated” hierarchical lattice model, with what turns out to be chaotic

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1In practice, however, the limitations of the procedure show up earlier, in the restriction of the partition function evaluation to only a subset of the full set of random bond configurations on the finite-volume lattice. See below.
real-space RG transformations, describes a spin glass. Intuitively this proposal is supported by the fact that under chaotic RG transformations the typical behavior is an essentially random jump between strong and weak coupling as larger and larger distance scales are probed, a behavior suspiciously reminiscent of a spin glass phase. Other circumstantial evidence also suggests a connection to chaotic phenomena [10], but difficulties in constructing reliable real-space RG transformations for spin glasses on Bravais lattices makes it difficult to establish a direct connection. For example, does spin glass behavior automatically entail chaotic real-space RG flows? Is the converse true?

As we shall suggest in this paper, there may be an indirect way of assessing the possible connection between chaotic RG flows and spin-glass behaviour. One striking consequence of the exact (chaotic) renormalization group transformations on hierarchical lattices is the limiting distribution of partition function zeros on, in general, fractal Julia sets [14]. If ordinary Bravais-lattice spin glass models are describable by similar chaotic RG transformations, an interesting possibility is that the fractal nature of the set of partition function zeros might be preserved. Certainly, if partition function zeros of certain spin-glass models turned out to form fractal sets in the thermodynamic limit, this would be a strong hint that the dynamics behind these models may be related to chaotic RG transformations. Can the argument be strengthened? The fact that hierarchical lattice models give rise to (in general, but not always, fractal) Julia sets for the partition function zeros is more general, and not tied directly to spin glass behaviour of the model under study. (Interestingly, partition function zeros on Julia sets can also arise due to approximations of exact real-space renormalization group transformations. For an illustration of this in the context of the 2-d Ising model, see ref. [15].) But the argument does run the other way: hierarchical models with frustration give spin glass behaviour, do have chaotic renormalization group transformations, and do indeed lead to partition function zeros lying on (in general fractal) Julia sets. One of the physical consequences of chaotic renormalization group transformations is that in general the free energy will have an infinite sequence of singularities [16]. This behaviour is again compatible with a scenario of partition function zeros falling on a fractal set in the complex temperature plane. We will discuss these issues in more detail in section 2.

Although the possibility of observing fractal behavior in the distribution of the partition function zeros served as the original motivation for the present work, we have in the process of investigation uncovered a number of perhaps unrelated but interesting facts about the Ising spin glass partition function zeros. Since the set of these partition function zeros for finite volumes appears to form a highly complicated geometrical domain in the complex temperature plane, it is important to unravel underlying regularities in the distribution. In particular, it would be desirable to be able to characterize the set of zeros by general class properties, as narrowly defined as possible. If we use as fundamental variable \( u \equiv \exp\left[ -2\beta \right] \) (where \( \beta = 1/T \) is the inverse temperature, generalized to the complex plane), the finite-volume partition function for an Ising spin glass is, for a fixed random bond distribution, a finite polynomial in \( u \). Instead of working with the partition function zeros themselves, we may therefore, equivalently, work directly with this polynomial.

While the distribution of zeros corresponding to the finite-volume partition function

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2Chaotic behavior may of course show up as artifacts of approximate RG transformations, without any physical significance [11]. In two dimensions, a regular renormalization group flow between fixed points of unitary, Poincaré invariant theories is ensured by Zamolodchikov’s c-theorem [12]. Spin glasses models can evade this theorem, since they do not satisfy the assumption of translation invariance. For a discussion of related issues, and some measurable predictions of chaotic RG flows, see ref. [8].
itself may be difficult to characterize in an exact manner, it may be possible to find (linear, if possible, but at least invertible) transformations that take the polynomial of the finite-volume partition function into new polynomials with zeros located in more simple domains. Characterizing the distribution of zeros of the transformed polynomials is equivalent to characterizing the finite-volume partition function zeros themselves. As examples, we show that certain linear transformations on polynomials, used in graph theory to classify graphs [17], can be used to transform the partition function zeros for arbitrary bond distribution into strikingly simpler geometric domains. For example, we will give an example of a transformation that, to the numerical accuracy we have available, maps all zeros of all our available samples onto the real line. Some of these transformations are described in section 3. These, or other transformations, may also provide alternative partial characterizations of the Ising spin glass partition functions, although the resulting transformed polynomial may not in itself have a thermodynamic interpretation as a partition function of a physical system.

Studying the partition function zeros of an Ising spin glass may on the surface seem to be a rather isolated problem. In fact, we shall argue on the contrary. Using the distribution of zeros in the complex plane of given complicated high-order polynomials (or even distributions of such polynomials, as in the present case) to classify or “reconstruct” various properties of the polynomials can be a tool of much wider generality, and may occur in many branches of science. We have already discussed the fact that precisely the same situation occurs in graph theory. In spin glass theory it gives a new, at the moment only numerical, handle with which to extract physical information about the infinite-volume partition function. Perhaps it may be amenable to analytical approaches as well. We hope to have convinced the reader about this point of view by the time we reach section 4, which contains our conclusions.

2 Random Polynomials and Spin Glasses

Consider the ±1 Ising spin glass, described by the finite-volume partition function

\[ Z_N(J, \beta) = \sum_{\{\sigma\}} \exp \left[ -\beta \sum_{i,\mu} (1 - J_{i,\mu} \sigma_i \sigma_{i+\mu}) \right] \] (1)

and the free energy

\[ F_N(\beta) = \frac{\sum \ln[Z_N(J, \beta)]}{\sum \{J\}} \] (2)

Here the sum on \( \sigma \) runs over all spin configurations where \( \sigma_i = \pm 1 \), \( J \) runs over all bond configurations with \( J_{i,j} = \pm 1 \) and \( \mu \) denotes the lattice translations defining the nearest neighbours. In the language of above, we have \( K_{ij} = \beta J_{ij} \). \( N \) is the number of sites, or volume, of the finite lattice defining the system. It is convenient for the present purposes to rewrite this partition function in terms of a sum over the energy degeneracies \( P_N(E) \), i.e. the number of states with energy

\[ E(\sigma) = \frac{1}{2} \sum_{i,\mu} (1 - J_{i,\mu} \sigma_i \sigma_{i+\mu}) \] (3)
on the given finite-size lattice. Then, introducing the variable \( u \equiv \exp[-2\beta] \), we have

\[
Z_N(J, u) = \sum_{E=0}^{N_b} P_N(E) u^E, \tag{4}
\]

where \( N_b \) is the number of bonds on the lattice.

A crucial observation is that for any finite volume \( N \), the relevant definition of partition function zeros in the quenched Ising spin glass case must consist of the accumulation of partition function zeros for each particular bond distribution. This follows directly from the definitions (2) and (4), which show that the quenched free energy

\[
F_N(u) = \ln\left[\prod_{\{J\}} Z_N(J, u)\right]/\sum_{\{J\}} \tag{5}
\]

behaves as if it had been obtained from an effective partition function of product form, once over each bond configuration. The effective partition function zeros can thus be computed in a step-by-step manner, one bond configuration at a time. For practical purposes, a sampling of configurations should provide enough information. Lee-Yang zeros and Fisher zeros have previously been computed numerically using this approach \[18, 3\] for 3-dimensional Ising spin glasses on lattices of varying finite sizes. Both kinds of partition function zeros hint, with the statistics available in those references, at an interesting structure in the infinite-volume limit.

A subtlety and possible weakness in the above line of reasoning ought to be mentioned at this point. Formally, in the infinite-volume limit, when all partition function zeros of all bond configurations \( \{J\} \) are considered, they will, in the above perspective, necessarily lead to physical singularities. Indeed, consider the “pure” Ising bond configuration, one of the bond configurations included in the infinite sum over \( \{J\} \). In the infinite-volume limit this model has a genuine singularity at a non-zero temperature for all dimensions larger than 1. Should this singularity, and its associated partition function zero be of special importance for the Ising spin glass? Naively, on the basis of eq. (5) the answer would be yes. But the flaw in this argument lies in the fact that not only does the free energy contain a piece given by the logarithm of all individual fixed bond configuration partition functions, it also contains the averaging over configurations. Clearly the Ising model partition function, and its associated partition function zeros, will be of “measure zero” in the total sum. But what about nearby models, partition functions with bonds that are almost pure Ising-like? If the density of partition function zeros of such models is large enough, it could lead to a singularity in the spin glass free energy. Whether it does or not, and where precisely a genuine singularity occurs in the free energy of the spin glass thus cannot be settled by looking at individual bond configurations, and just tracing the location of the associated partition function zeros. It is only the total sum of all zeros that is meaningful, and here some notion of regularization is required. Indeed, the above state of affairs illustrates a potential difficulty with a proper definition of the spin glass effective partition function from the limit (as the volume is sent to infinity) of all bond configurations in a finite volume, using eq. (5). A perhaps not unrelated problem is, in more physical language, that as the volume is increased, there may be new ground states at every new length scale. In mathematical terms, the strict definition of the infinite-volume spin glass effective partition function (5) may require a proper regularization (zeta-function regularization, or otherwise), and this regularization may shift the eigenvalues of the transfer matrix away from their naive values.
Basically, what can happen is that the naive location of a zero in the factorized infinite product (5) may occur at a point in the complex plane where the remaining infinite product fails to converge. In this manner a divergence and a potential zero can compensate each other, producing a displaced zero. This is a problem inherent to defining the effective spin glass partition function itself in this manner, instead of relying on the indirect quenched-average prescription. We will have nothing new to say about it. We will simply take it for granted that a finite-volume study of this model is meaningful in the sense that it may yield, by extrapolation, information about the eventual object of study, the infinite-volume partition function itself.

For a given bond distribution \( \{J_{ij}\} \), the finite-volume partition function \( Z_N(J, u) \) is a polynomial of degree \( n \leq N_b \) in the variable \( u \). The coefficients \( P_N(E) \) of this polynomial are drawn from a probability distribution determined by the random bond distribution \( \{J_{ij}\} \). This is an example of what in the mathematical literature is known as a random polynomial \[19\]. Although distribution of zeros of various classes of random polynomials with continuous coefficient distributions has been the subject of much study (see, e.g., ref. \[19\]), few results are known for random polynomials with discrete distributions of coefficients, and none for the particular distribution \( P_N(E) \) obtained from the expansion (4). (For a comprehensive discussion of mathematical results concerning the location of zeros of polynomials, see also ref. \[20\].) Clearly, we can view our problem from a more general perspective, and it is tempting at this stage to consider a “number-theoretic partition function” \( Z_N \) and a “free energy” \( F_N(\beta) \) by the definitions (4) and (2) for any distribution of coefficients \( P_N(E) \), not necessarily related to any statistical mechanics problem. In this context, the index \( N \) would rather denote a given (arbitrary) way of restricting the possible coefficients and degrees. In particular, one can imagine deforming the Ising spin glass partitions by choosing the coefficients \( P_N(E) \) from a distribution close, but not exactly equal, to that of the Ising spin glass. Such generalizations may be of interest in their own right, but we will consider them here only to get a preliminary idea of what kind of distribution of partition function zeros we may expect for the true Ising spin glass. The enormous advantage of choosing a deformed distribution for \( P_N(E) \) is that we can supply it by hand, thus avoiding the precise determination of the Ising spin glass partition function for all given bond distributions. Such an approach has in fact been suggested earlier by Derrida \[22\] in the special case of a gaussian distribution, where it is known as the random energy model. In what follows, we will examine the zeros of related classes of polynomials whose features make them more and more similar to an Ising spin glass partition function for a generic bond configuration. The similarities as well as differences observed at the level of the zeros will help in understanding the specificity of the Ising glass case.

### 3 Distribution of Zeros

To get some preliminary idea of what kind of distribution we can expect for random polynomials with positive integer coefficients, let us first consider the class of polynomials with a bound on the degree, \( N_{\text{max}} \), and a common bound on the coefficients \( C_{\text{max}} \). Shown in fig. 1 is: (a) a representative plot of zeros of random polynomials with \( N_{\text{max}} = 4 \) and \( C_{\text{max}} = 6 \); (b) \( N_{\text{max}} = 10, C_{\text{max}} = 5 \); (c) \( N_{\text{max}} = 10, C_{\text{max}} = 100 \); (d) \( N_{\text{max}} = 30, C_{\text{max}} = 5 \) (in this last case setting all odd coefficients to zero, for reasons explained below).

The first remarkable fact is that the zeros are not uniformly spread in the complex plane,
but are centered around the unit circle. Also, there are clearly defined zones of much higher density, their number corresponding exactly to the value of the bound on the degree. Both features have proven to be generic, at least in all the cases we have examined. It will turn out that it takes very particular distributions of coefficients to deviate from this general pattern. Another remarkable feature is the presence of holes centered at roots of unity. Let us study the evolution of this feature as we relax the bound on the coefficients of the random polynomial. Figures 1b and 1c show that when we increase the range of the allowed coefficients, the average size of the holes tends to decrease, but one can keep on tracing them on a smaller scale.

In fact, in the very special case of $C_{\text{max}} = 1$, it could be proved that all zeros of all random polynomials within that particular class are enclosed within a narrow region (the exact definition of which can be found in ref. [23]) around the unit circle in the complex plane. The results of that paper are of particular interest to us, and we shall frequently refer to it in what follows.

Figure 2a shows the situation for $N_{\text{max}} = 18$, and figure 2b is a blown-up region of it, in both cases having $C_{\text{max}} = 1$. The original figures of ref. [23] are of higher quality, but we include our versions of them in order to be able to compare later with our corresponding figures for spin glasses. Note that there is a tendency of the zeros to accumulate on minute segments of arc-like curves, giving the pictures a highly non-trivial appearance, especially at the borders of the set. It gets quickly impractical to obtain a higher density of points in these regions, as the corresponding polynomials seem to be fairly rare among all the others. In the work of Odlyzko and Poonen [23], the study of these features could nonetheless be pursued much further by using a reverse procedure which is directly tied with that particular distribution of coefficients. Instead of explicitly computing the zeros of polynomials, the authors systematically tested if, conversely, a given point in the complex plane could be a zero of some random polynomial belonging to the case $C_{\text{max}} = 1$, hereafter denoted the 0-1 class. This was based on a cascade of inequalities peculiar to the 0-1 case. Working at the maximal resolution of their printer, it enabled them to provide spectacular evidence that the limiting set of the zeros, when the degree is arbitrarily large, corresponds to a fractal. Odlyzko and Poonen could also provide a heuristic explanation of the self-similarity at the analytical level, but again, this seems to be possible only because of the specificity of the 0-1 situation. Nonetheless, we regard these results as important also for our case, because they illustrate, among others, how a fractal structure of zeros of a given class of polynomials can emerge in a practical numerical study. It was thus important to include our versions of the Odlyzko-Poonen figures obtained by the brute-force approach, although we here to great advantage could have used the reverse procedure. The direct method is the only way we have available to tackle more complicated classes of polynomials (in particular, those related to spin glasses).

Of course, we are not expecting that any discrete distribution of coefficients will lead to a fractal distribution of the zeros. One interesting and relevant counterexample is precisely the case of the random energy model [22]. Here the coefficients $P_N(E)$ in eq. (4) are chosen according to a Gaussian distribution. This leads to an essentially solvable model, and interestingly also the distribution of partition function zeros can be computed exactly [24]. It turns out to be a regular (non-fractal) set in the complex plane, which also, to the statistics available, has been observed in numerical analyses [25]. So spin-glass behaviour may certainly not in itself necessarily imply a fractal set of partition function zeros. With this perspective in mind, let us now turn to the results of the present investigation concerning
3.1 The Ising spin glass zeros

We will here present some examples of the sets of zeros corresponding to genuine Ising glass partition functions. We have obtained numerous plots of partition function zeros, for a wide range of lattice sizes, mostly in 2 dimensions, but also some in 3 dimensions. The figures we have selected here are the most illustrative of the generic features we have observed. Before commenting on the pictures, let us explain how the partition functions themselves have been obtained. The method we used has previously been described in ref. [3], so we shall only briefly outline the main idea (for a different approach, see ref. [4]).

For a given bond configuration \( \{ J_{ij} \} \), the partition function is evaluated exactly using a numerical transfer matrix technique [26], which recursively updates the partition function while building up the \( D \)-dimensional lattice, stacking \((D - 1)\)-dimensional slices one by one. In [3], the finite geometries of the lattices so obtained were chosen to correspond to “helical boundary conditions”, which minimized the finite-size errors in the derivation of the corresponding low-temperature series. In our present case, where global topological properties of the set of zeros, and its dynamics with increasing \( N \), are of primary interest, we will assume that the boundary conditions are of second importance. One has only to pay attention to the correct scaling of the size of the lattice, so that it defines a constantly \( D \)-dimensional pattern, and does not degenerate into one of smaller dimension. Only under these conditions, a finite-size scaling analysis of the location of the zeros can be meaningfully undertaken. But such a finite-size scaling analysis will not be performed in our present study, where we in fact have mostly used helical lattices. They can be defined in the following way (for a more complete treatment, the reader is urged to consult ref. [27]). Consider sites numbered sequentially with integers, and, for a system of dimension \( D \), a set of \( D \) integer “periods”: \( h_1 \leq h_2 \leq \ldots \leq h_D \), so that the nearest neighbours of a site \( i \) in the direction \( j \) are defined by the jumps \( i \pm h_j \). The biggest period \( h_D \) can be viewed as defining one “turn” of a helix. The total helical (finite) lattice is then built up from superposing the desired number of such turns. The corresponding partition function (for a given bond distribution \( J \)) is obtained by the recursive procedure described above. Helical lattices of this type are locally hypercubic, but their global geometry is topologically more involved. Their resulting behaviour, as far as distribution of zeros is concerned, should, however, be qualitatively similar to those of more conventional periodic hypercubic lattices.

We have mainly considered 2-dimensional models where we could more efficiently gather a substantial number of data points. However, consideration of some 3-d cases showed that they exhibit similar features at the level of their distribution of zeros. Typically, the number of points per plot is of the order of 100,000 (which was also the case for the previous figures). Our algorithm checked that the zeros generated by one random bond configuration did not reproduce the zeros already obtained. In our lattices, each site is connected to 2d neighbours, which causes all \( P_N(E) \) with \( E \) odd to vanish, as can be easily proved. The resulting distributions of zeros have consequently symmetry both about the real and the imaginary axis. It is thus sufficient to examine only what happens in the first quadrant of the complex plane. Figures 3a-d all deal with the 2-d Ising spin glasses. Lattice sizes are (a) \( N = 18, h_2 = 7 \), (b) \( N = 18, h_2 = 3 \), (c) \( N = 18, h_2 = 3 \), (d) \( N = 18, h_2 = 6 \), and (e) \( N = 19, h_2 = 3 \), the figure 3c showing finer details of 3b. The very first striking fact is the dissimilarity with the figures 1 and 2. Instead of a high concentration on the unit circle, and
almost void interior region, the contrary seems to occur here. This is troubling, because, taking the bound on the coefficients sufficiently high, the flat distributions of the preceding section are generating, among others, all genuine Ising glass polynomials. It seems then that the latter must be particularly scarce. Indeed, for a given volume \( N \), the maximal degree of the spin glass partition function is \( N_b = 2N \), and the bound on the coefficients is certainly grossly overshot by \( 2^N \). There are then \( 2^{N(N_b+1)} \) random polynomials, which contain in particular the \( 2^{2N} \) spin glass partition functions. However, this does not explain why the zeros of the Ising spin glass partition functions do not tend at all to accumulate around the unit circle, despite the fact that this generically is the most dense region. To understand the situation better, one can first examine the effect of setting to zero, in the flat case, all the odd coefficients. Figure 1d already showed that this restriction does not explain the dissimilarity. If one examines the Ising glass partition functions, another feature is apparent. For any bond distribution, there seems to exist an index \( E_0 \) such that \( P_N(E) < P_N(\bar{E}) \) for \( E < \bar{E} < E_0 \) and \( P_N(E) > P_N(\bar{E}) \) for \( E > \bar{E} > E_0 \), where only non-vanishing coefficients are considered. Sequences of integers with this property are well known in combinatorics and graph theory where it is called unimodality. In all configurations we have studied, we have never encountered any violation of unimodality, but we have no direct proof that in fact all Ising spin glass distributions have this property.

The next obvious step is then to deform the flat distributions considered above in such a manner that unimodality is incorporated. Figure 4a shows the result for polynomials with \( N_{\text{max}} = 30, C_{\text{max}} = 100,000 \) where all odd coefficients are set to zero, and where unimodality instead is being implemented in the following manner. We take, for a random number \( r \) flatly distributed between 0 and 1, the remaining even coefficients \( N_{k+2} = N_k r(C_{\text{max}} - N_k) \) up to the “middle” coefficient. Past this point we take \( N_{k+2} = N_k r \). We see that we get closer to the pictures of figure 3, albeit this does not seem to be the end of the story. To more drastically remove zeros from the unit circle, and place them closer to the interior region, consider figure 4b, which show the corresponding zeros with \( N_{k+2} = (N_k r)^\alpha \) (\( \alpha \) being a flatly distributed random number between 1 and 2) up to the middle of the polynomial, the procedure being mirrored for the remaining \( N_k \)‘s, i.e. such that

\[
N_{N_{\text{max}}-2k} = N_{2k}.
\]

It looks as if this exponential growth of the coefficients better “simulates” the Ising spin glass case. But clearly other “correlation” effects among the coefficients, much harder to characterize, are important as well.

It can be shown that for helical lattices with \( N \) even, \( h_1 = 1 \) and \( h_2 \) odd, for each spin configuration of energy \( E \), there exists another configuration of energy \( N_b - E \). This means that the corresponding partition function has the mirror symmetry \( P_N(E) = P_N(N_b - E) \). As a consequence, if \( x_0 \) is a zero, then so is \( 1/x_0 \). This feature is not generic, and of course does not explain the suppression of zeros around the unit circle. Furthermore, the structure of the fine details of the zeros (and particularly around the boundaries) is not affected by imposing this mirror symmetry, cf. figure 3d, which is not mirror-symmetric.

Apart from these global aspects, a closer look at the zeros of actual Ising spin glass partition functions reveals that, remarkably, many of the small-scale features of the 0-1 case are present here too. The zeros tend to coagulate, and, at the boundaries, the same “spike” or “cusp”-like organization seems to take place. This is especially evident in figures 3c and 3d, which display distinct fractal-like features along the boundary. Although it is far from conclusive, the similarity of these boundary features with the ones present in the
known fractal case of \cite{23} (compare figure 2) certainly makes the hypothesis that the Ising spin glass partition function zeros may accumulate on a fractal set a genuine possibility.

4 Graph Theory and Polynomial Mappings

As it turns out, some of the mathematical machinery used in graph theory to classify graphs can with advantage be applied to Ising spin glass theory as well. Although there seems to be no direct mapping between finite-volume Ising spin glass partition functions and particular graphs, certain transformations of polynomials used in graph theory may be useful here as well.

Since most of the notions we will be borrowing from graph theory are not readily available in the physics literature, we begin with a few definitions. In graph theory, one can associate to each graph $G$ a polynomial, the chromatic polynomial $P(G; x)$, first introduced by Birkhoff. We do not need its precise definition in terms of a given graph (for a good introduction to the subject, see ref. \cite{17}), but it is important that it can be represented by an expansion

$$P(G; x) = \sum_{j=0}^{n} a_j(G)(x)_j,$$

with non-negative integer coefficients $a_j$. Here,

$$(x)_j \equiv x(x-1) \cdots (x-j+1)$$

is known as the $j$-th falling factorial polynomial, and $n$ is the number of vertices of the graph. The coefficients $a_j$ of the expansion (7) have a direct interpretation in terms of partitions of vertices of the graph; $a_j$ is the number of inequivalent way of dividing the vertices of the graph $G$ into exactly $j$ blocks, each inducing what in graph theory is known as an edge-free subgraph of $G$ (see ref. \cite{17}). It is then easy to see that, for an integer $k$, $P(G, k)$ gives the number of proper colourings of the graph $G$ using $k$ colours.

One important property of the chromatic polynomial is related to its expansion in the $x^j$-basis instead of the $(x)_j$-basis used in the definition (7) above. It is readily shown that in this basis the coefficients are alternating in sign, so that we may introduce non-negative integer coefficients $b_j$ defined by

$$P(G; x) = \sum_{j=0}^{n} (-1)^{n-j} b_j(G)x^j.$$  

The coefficients $b_j$ have been conjectured to be not only unimodal,

$$b_0 \leq \cdots \leq b_k \geq \cdots b_n,$$

for some index $k$ (with $0 \leq k \leq n$), but in fact strictly logarithmically concave:

$$b_j^2 > b_{j-1}b_{j+1}.$$ 

It is precisely this conjecture which, among others, motivates the study of the zeros of the chromatic polynomials. Also, the location of the zeros of the polynomial can be used

\[3\]Most of the presentation below follows the excellent exposition in ref. \cite{21}.\]
as a criterion in the “reconstruction” or “inverse” problem which consists in examining the conditions upon which a given polynomial can be a chromatic polynomial of some graph. Although necessary conditions are relatively easy to derive (see [17]), sufficient ones are not known in general. Researchers in this field are therefore confronted with problems which are quite similar in nature to those met in our present study. In general a class of polynomials obtained by an explicit process is studied from the point of view of their zeros, but the process itself gets quickly too complex to enable a direct investigation of the general case. The only possibility is then to remain within small volumes or, in the language of graph theory, a small number of vertices. Here computer algorithms can be used. One may therefore hope that techniques which have proven useful in one field may be successful in the other as well. What follows is devoted to examining one such possibility, based on recent results in [21].

The zeros of general chromatic polynomials, although bounded in several ways in the complex plane, fall in highly irregular regions. But certain associated polynomials, directly derivable from the chromatic polynomial itself, have zeros that display striking regularities. Given a chromatic polynomial \( P(G; x) \), one can introduce three related polynomials that are particularly useful: the \( \sigma \)-polynomial, the \( \tau \)-polynomial, and the \( \omega \)-polynomial. These are defined as follows [21]. The \( \sigma \)-polynomial is obtained from the chromatic polynomial by taking the number of partitions \( a_j(G) \) of eq. (7) as fixed coefficients, but replacing the basis \( (x)_j \) by the basis \( x^j \). Thus,

\[
\sigma(G; x) = \sum_{j=0}^{n} a_j(G)x^j,
\]

which obviously should not be confused with the expansion of the chromatic polynomial itself in the \( x^j \)-basis, eq. (9).

To construct the \( \tau \)-polynomial, first expand the chromatic polynomial \( P(G; x) \) in the \( (x)_j \)-basis as well:

\[
P(G; x) = \sum_{j=0}^{n} (-1)^{n-j}c_j(G)(x)_j,
\]

where

\[
(x)_j \equiv x(x+1)\cdots(x+j-1)
\]

is the \( j \)-th rising factorial polynomial. Then define the \( \tau \)-polynomial by taking the coefficients \( (-1)^{n-j}c_j \), but replacing the basis \( (x)_j \) by \( x^j \), viz.,

\[
\tau(G; x) = \sum_{j=0}^{n} (-1)^{n-j}c_j(G)x^j.
\]

Finally, introduce the \( \omega \)-polynomial by

\[
\omega(G; x) = \sum_{j=0}^{n} h_j(G)x^j = (1-x)^{n+1}\sum_{m} P(G; m)x^m,
\]

where the sum in the last expression runs over all natural numbers. The last identity in eq. (16) is highly non-trivial, but not very useful from a practical point of view. Fortunately, a
number of identities exist, which relate the different polynomials to each other and to more manageable expressions. For example, one can show \[21\] that

\[
\omega(G; x) = (1 - x)^n \sum_{j=0}^{n} j! a_j(G) \left( \frac{x}{1 - x} \right)^j. \tag{17}
\]

This last identity hints at the usefulness of introducing what are called augmented \(\sigma\) and \(\tau\) polynomials, which will be denoted by \(\bar{\sigma}(G; x)\) and \(\bar{\tau}(G; x)\), respectively:

\[
\bar{\sigma}(G; x) = \sum_{j=0}^{n} j! a_j(G) x^j, \tag{18}
\]

and

\[
\bar{\tau}(G; x) = \sum_{j=0}^{n} (-1)^{n-j} j! c_j(G) x^j. \tag{19}
\]

In particular, note that

\[
\omega(G; x) = x(1 - x)^n \bar{\tau} \left( G; \frac{1}{1 - x} \right). \tag{20}
\]

There are a number of interesting functional identities between the different polynomials, and the original chromatic polynomial. They can be useful because they may establish connections between the original finite-volume Ising spin glass partition function and some of the new polynomials derived from it.

The four polynomials \(P(G; x), \sigma(G; x), \tau(G; x)\) and \(\omega(G; x)\) can be used to generate an interesting hierarchy of conditions regarding “reality” of the polynomials (a polynomial is defined to be real if all its roots are real) \[21\]. These reality conditions are of an entirely general nature, and can hence be used for arbitrary polynomials, including the ones that have a physical meaning as Ising spin glass partition functions in a finite volume. To quote some examples: \(\omega\)-reality implies both \(\sigma\)-reality and \(\tau\)-reality. \(P\)-reality implies \(\tau\)-reality, and the conditions \(P\)-reality, \(\tau\)-reality, \(\omega\)-reality and \(\sigma\)-reality all imply that the corresponding \(P, \tau, \omega,\) and \(\sigma\) polynomials have coefficients that form a strictly logarithmically concave sequence. Of course, for polynomials based on both graph theory chromatic polynomials and finite-volume Ising spin glass partition functions there may be further specific relations that are valid only within these subclasses.

To demonstrate how these mappings can be used in our Ising spin glass case, consider identifying

\[
P_N(E) = a_E, \tag{21}
\]

so that the actual partition becomes the \(\sigma\)-polynomial (of course with only even coefficients, so there is certainly no graph corresponding to it). Let us now compute the zeros of the associated \(P\)-polynomial. This is shown in figure 5a, for a lattice of \(N = 12, h_1 = 1, h_2 = 7\). As another example, consider the \(\bar{\tau}\)-polynomial derived again from the same identification; we show the zeros of this polynomial for \(N = 17, h_1 = 1, h_2 = 5\) in figure 5b. (This is particularly interesting, because the pure Ising model treated in the same manner yields a set of zeros that appears to form a perfect ellipse.) Although we are not showing it (because it has no structure whatsoever), perhaps the most interesting plot is that of the zeros of the the \(\tau\)-polynomial itself. Here, for all Ising spin glass partition functions we have considered, all
zeros fall \textit{exactly} on the real axis. The Ising spin glass partition functions thus appear, to the extent we have been able to sample them, to be $\bar{r}$-real.\footnote{An interesting check concerns the application of these polynomial maps to an exactly solvable case such as the ordinary 1-d Ising model. Using explicit representations of the finite-volume model (see, e.g., ref. \ref{28}), we have confirmed that the properties of the mapped polynomials are shared by this particular model. These mappings may be of use also for the study of higher-dimensional Ising models.}

We consider the transformations of polynomials described above as just examples of what might be useful tools for analyzing the original partition function zeros. The polynomials we have considered here do have a number of almost magical properties when defined from an original polynomial with integer (or rational) coefficients, and in that sense several of the properties discussed above are of a far more general nature, and are not restricted to random polynomials of distributions corresponding to Ising spin glasses. Ideally, one should find transformations such that the transformed polynomial satisfies a certain criterion concerning its zeros (such as reality) \textit{only} in the class of random polynomials that correspond to Ising spin glass partition functions. Evidently, the broader the class, the less suited it will be for a classification of the Ising spin glass partition functions. But the examples we have given above certainly do share a number of useful properties, and it is not unlikely that new related transformations can be used to further limit the class of polynomials for which the zeros form simple patterns in the complex plane.

\section{Conclusion}

We hope to have convinced the reader at this point that an analysis of the distribution of zeros of Ising spin glass partition functions is important. This is a subject of study which has become possible within the last few years due to the increased computational power available, and it has revealed a number of very interesting facts about the Ising spin glass partition function. At a detailed numerical level, the approach towards the real temperature axis can give information about the nature of the spin glass phase transition, and about its critical exponents. In this paper we have argued that \textit{global} aspects of the distribution of zeros can contain highly non-trivial information as well. Although all of our analysis is numerical at this point, we have presented visual evidence that the full distribution of partition function zeros is forming a highly non-trivial set in the complex temperature plane. Whether this set actually is fractal cannot be proved at this level, but it clearly remains a genuine possibility. If correct, this would indirectly provide an intriguing hint that the underlying renormalization-group dynamics may be chaotic, a connection so far only established in the perhaps more contrived spin glass models defined by spin systems with frustration on hierarchical lattices.

We have tried to show that there may be more analytical means of studying this problem as well. In particular, finding appropriate polynomial transformations may be the tool with which the highly complicated distribution of partition function zeros can be brought under much tighter control. It is plausible that a very specific polynomial mapping exists, which uniquely selects out Ising spin glass partition functions as those members of a class of random polynomials whose zeros, when considered in the transformed basis, fall on very simple domains (such as the real line). In section 4 we gave various examples of candidates for such polynomial mappings, thereby making a (perhaps fortuitous) connection to Graph Theory. These mappings fail, however, to be sufficiently selective for our purposes.
Instead of relying on visual evidence, a direct way to test whether the set of partition function zeros of the Ising spin glass fall on a set of fractal dimension is of course to compute this dimension on the basis of our data. Such a procedure is, however, not free of ambiguities. First, the notion of a fractal dimension is in itself not unique (there are infinitely many ways of “analytically continuing” the common definition of integer dimensions to the set of reals), and second, extracting the fractal dimensions in this way on the basis of raw data alone is highly non-trivial. The non-uniqueness of the notion of a fractal dimension is often, arbitrarily, parametrized within one given class of fractal dimensions in terms of one real number \( q \). This definition, which dates back to the work on the entropy of probability distributions by Rényi, starts by subdividing the space (in this case the complex temperature plane) into a more and more fine grid of linear size \( r \). Let \( p_k \) denote the probability that an element of the set is contained within the \( k \)'th cell. The generalized fractal dimensions \( D_q \) is then defined by

\[
D_q \equiv \lim_{r \to 0} \frac{1}{q-1} \ln \left[ \frac{\sum_k p_k^q}{\ln(r)} \right]
\]  

(22)

for all \( q \neq 1 \). For \( q=1 \), the analogous definition is

\[
D_1 \equiv -\lim_{r \to 0} \frac{p_k \ln(p_k)}{\ln(1/r)}.
\]  

(23)

This latter, \( D_1 \), is known as the information dimension. \( D_0 \) is the more commonly known Hausdorff dimension, and \( D_2 \) is denoted the correlation dimension in the literature.

While it is not obvious which fractal dimensions \( D_q \) (or others) one should focus on, a more practical problem concerns the actual determination of these numbers \( D_q \) from our raw data. Although several of our samples of partition function zeros contain as many as 100,000 points, this number is in fact not sufficient to determine reliably the limit \( r \to 0 \) in eq. (22). The subdivision of intervals leads to an exponential growth in cells, which quickly clashes with the requirement that the typical number of points per filled cell should be larger than one. Thus one quickly reaches a regime (as a function of subdivisions of the cells) where one is only measuring the thinning-out of points due to the finite sample. We have attempted to calculate both the standard Hausdorff dimension \( D_0 \) and the correlation dimension \( D_2 \) in this brute-force manner, but will not quote any numbers, since they are too inconclusive. The only statement we can make is that a Hausdorff dimension of two for the interior of the set is not incompatible with our results.

How can the issues brought up by the present paper be studied in greater detail? There are severe numerical limitations in going significantly beyond the number of computed partition function zeros (or, equivalently, the lattice sizes that we have reached). Increasing the number of data points 10-fold, perhaps 100-fold, may be what is required to really see a possible conclusive fractal structure emerging, as the 0-1 case discussed in section 3 has indicated. It may even be that, deviously, an apparent fractal behaviour seems to emerge on smaller systems, but disappears in the limit of the volume going to infinity. Clearly, the converse procedure, an algorithm that can tell (to any given accuracy) whether a point in the complex plane can belong to the zeros of Ising spin glass partition functions or not would therefore be highly advantageous. Finding such an algorithm is, however, far more difficult than the 0-1 case referred to above. In fact, the availability of such an algorithm would almost amount to having an explicit solution for Ising spin glass partition functions of arbitrarily large volumes.
Another aspect that deserves further study in the light of our findings, is the distribution of Lee-Yang zeros in the complex activity plane. The very preliminary results reported in ref. \[18\] certainly hint at an analogous structure present in the set of those zeros. With present-day computers this aspect of spin glass theory can be pushed much beyond the results known so far.

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Note Added: After the completion of this paper, we became aware of the recent work by Baake, Grimm and Pisani \[29\]. These authors demonstrate that a spin model defined on a regular lattice can lead to a fractal distribution of partition function zeros. To our knowledge, this is the first time it has been demonstrated that fractal sets of partition function zeros can arise in models other than those defined on hierarchical lattices. The model they consider is a one-dimensional Ising-like theory with fixed nearest-neighbour couplings that are distributed according to a Fibonacci sequence.

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Figure Captions

**Fig. 1a)** Distribution of zeros of random polynomials of degree 4, with all coefficients taken randomly from a flat distribution between 1 and 6. There is a slight increase in the density of points around four spots close to the unit circle. There are also distinct holes in the distribution close to points on the unit circle.

**Fig. 1b)** Same as fig. 1a, but this time the degree of the random polynomial is increased to 10, and the coefficients are sampled randomly between 1 and 5. There are ten clear regions along the unit circle where the density is markedly larger. The holes have shrunk in size.

**Fig. 1c)** The degree is still 10, but the range of the coefficients is now increased to the interval [1,100]. The ten regions of higher density along the unit circle clearly remain, but the holes have decreased in size.

**Fig. 1d)** The random polynomial is taken with only *even* powers. We show here an example of degree 30, with coefficients taken randomly in the interval [1,5]. The number of regions of higher density is fourteen, one less than the generic fifteen for a random polynomial of degree 30. The holes along the unit circle can still be seen.

**Fig. 2a)** Zeros in the upper complex plane of random polynomials of degree 18 and coefficients 0 or 1.

**Fig. 2b)** Finer details of the fig. 2a-case. The distribution is believed to be fractal.

**Fig. 3a)** Partition function zeros of a 2-d Ising spin glass of the form discussed in the text. Here $N=18, h_1=1, h_2=7$.

**Fig. 3b)** Same as in fig. 3a, but with $h_2=3$.

**Fig. 3c)** Blown-up picture of the partition function zeros displayed in fig. 3b.

**Fig. 3d)** Partition function zeros when for the same lattice above we set $h_2=6$. For this lattice size there is no reflection symmetry with respect to the unit circle (such that when $x_0$ is a root, so is $1/x_0$). The fine details of the distribution of zeros is, as would be expected, unaffected by this symmetry.

**Fig. 3e)** Details of the distribution of zeros for a slightly larger lattice with $N=19, h_2=3$, which again does not have symmetry with respect to inversions around the unit circle.

**Fig. 4a)** In order to mimic the basic features of the spin glass partition function zeros, we here consider random polynomials with a distribution of coefficients of linear growth (until the middle of the polynomial, and a linear decrease beyond the middle), as explained in detail in the main text. It is clear that the generic tendency of the zeros of random polynomials to accumulate close to the unit circle has been modified. There is a shift toward the interior of the unit circle. The polynomials are of degree 30, with a distribution of coefficients between 1 and 100,000.

**Fig. 4b)** Same as fig. 4a, but this time choosing an even steeper rise in coefficients until the middle of the polynomial, and a corresponding steeper decrease beyond the middle. The exact distribution is described in the main text. Note that the zeros have been shifted completely away from the unit circle, mimicking many of the gross features of the genuine Ising spin glass case.

**Fig. 5a)** Example of how the zeros of the Ising spin glass partition function look in a “transformed basis”, as described in the main text. Shown here is the distribution of the zeros of the associated $P$-polynomial (the analogue of the chromatic polynomial in graph theory). The original Ising spin glass lattice corresponds to $N=12$.

**Fig. 5b)** Ising spin glass partition function zeros in the $\tilde{\tau}$-picture, here for a lattice of $N=17$. 

Page 18