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COMBINATORIAL PROBLEMS ARISING FROM THE STATISTICAL MECHANICS MODEL OF SPIN GLASSES

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Abstract. A problem of calculating the free energy of the Ising spin glass model on a graph is reformulated into certain combinatorial enumeration problems.

1. Introduction

Spin glasses are magnetic systems in which the interactions between the magnetic moments are "in conflict" with each other due to some frozen-in structural disorder ([1]). The Ising spin glass model, which is the subject of this paper, is a statistical mechanics model for such magnetic systems. To take account of the disordered nature, interactions are assumed to be random variables and the averaging over these variables is taken for the free energy. The computation of the averaged free energy is the aim of statistical mechanics of spin glasses.

We consider the Ising spin glass model on a general graph G (see Section 2). We shall give two differnt reformulations for the free energy of the model: one of which is based on the high-temperature expansion (Section 3), and the other based on the low-temperature expansion (Section 4). The both formulations rely on the replica trick ([4],[2]) and convert the original problem into certain combinatorial enumeration problems. To demonstrate how they work, we shall give explicit computations for the model on the cyclic chain (Section 5).

In condensed matter physics the graph G (the *base space* of the model) is (almost) always assumed to have some symmetry, such as translational one. From such a physics viewpoint the simplest but nontrivial one is the model on the two-dimensional square lattice with cyclic boundary conditions, for which the exact solution has not yet been obtained; this is an open problem.

2. The Ising spin glass model

Let G be a graph, consisting of a finite set V of points (or vertices), $\#V = N$, and a finite set B of edges (or bonds), $\#B = M$. We assume that G is simple;

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that is, G has no loops or parallel edges. Then each edge can be specified as (α, β) by its distinct endpoints. To each point $\alpha \in V$ attach the set $\{-1, 1\}$, and call a cross-section $\sigma : V \to \{-1, 1\}^N$ a spin configuration. Let $\mathbb{C}$ be the set of all spin configrations. For a given $\sigma \in \mathbb{C}$ and $\alpha \in V$ we call $\sigma_\alpha = \sigma(\alpha)$ the (value of) spin on the point α. To each $(\alpha, \beta) \in B$ let us attach a real parameter $K_{\alpha\beta}$ which specifies the interaction between adjacent spins on α and β. The partition function of the Ising model on G for the interactions $\mathbf{K} = (K_{\alpha\beta} | (\alpha, \beta) \in B)$ is, by definition,

$$Z(\mathbf{K}) = \sum_{\sigma \in \mathbb{C}} \exp\Big(\sum_{(\alpha,\beta) \in B} K_{\alpha\beta} \sigma_\alpha \sigma_\beta \Big). \tag{1}$$

One of the goals in statistical mechanics is to compute the free energy per point

$$f(\mathbf{K}) = -\frac{T}{N} \log Z(\mathbf{K}).$$

This is the definition of the Ising model for given interactions $\mathbf{K}$ on the graph G. (Cf. such general models were considered in [3] by the author).

Now let us introduce randomness in the interactions $\mathbf{K}$. We assume that each $K_{\alpha\beta}$ takes values $\pm K$ with equal probability independently, where $K > 0$ is a parameter whose physical meaning is $K = J/T$ where J is the coupling constant and T the temperature. Observed (physical) free energy in the spin glass system is supposed to be the average

$$\langle f(\mathbf{K}) \rangle_{\mathbf{K}} = \frac{1}{2^M} \sum_{\mathbf{K} \in \mathbb{K}} f(\mathbf{K}) = -\frac{T}{N} \langle \log Z(\mathbf{K}) \rangle_{\mathbf{K}} \tag{2}$$

where $\mathbb{K}$ is the set of all $\mathbf{K} : B \to \{-K, K\}^M$. In statistical mechanics this average is called an quenched average. (For more physics background we refer to a review [1].) Thus our task is the computation of $\langle \log Z(\mathbf{K}) \rangle_{\mathbf{K}}$.

In the next two sections we will give two different reformulations of $\langle \log Z(\mathbf{K}) \rangle_{\mathbf{K}}$: either of which converts the problem to that of calculation of a generating function of a certain enumeration problem on the graph G (or its dual). In both cases, to compute the average of $\log Z$, we will use the *replica trick* ([4],[2]): that is, we will use the exact relation

$$\langle \log Z \rangle = \lim_{n \to 0} \frac{1}{n} \big(\langle Z^n \rangle - 1 \big) = \lim_{n \to 0} \frac{\partial}{\partial n} \langle Z^n \rangle.$$

3. Reformulation based on the high-temperature expansion

The first reformulation of (2) is based on the so-called high-temperature expansion. Substituting

$$\exp(K_{\alpha\beta} \sigma_\alpha \sigma_\beta) = (\cosh K_{\alpha\beta})(1 + \sigma_\alpha \sigma_\beta \tanh K_{\alpha\beta})$$

(since $\sigma_\alpha \sigma_\beta = \pm 1$) we can rewrite (1) as

$$Z(\mathbf{K}) = \Big(\prod_{(\alpha,\beta) \in B} \cosh K_{\alpha\beta} \Big) \sum_{\sigma \in \mathbb{C}} \prod_{(\alpha,\beta) \in B} \big(1 + \sigma_\alpha \sigma_\beta \tanh K_{\alpha\beta} \big). \tag{3}$$

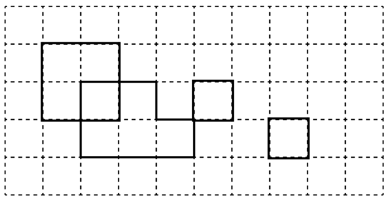
Expanding the summand, taking the summation $\sum_{\sigma\in\mathbb{C}}$, and noting that

$$\sum_{\sigma_\alpha=\pm 1} \sigma_\alpha^k = \begin{cases} 2 & \text{for } k \text{ even,} \\ 0 & \text{for } k \text{ odd,} \end{cases}$$

we have an expression in terms of *polygons* (defined below)

$$Z(\mathbf{K}) = 2^N \Big(\prod_{(\alpha,\beta)\in B} \cosh K_{\alpha\beta} \Big) \sum_{P\in\mathbb{P}} \prod_{(\alpha,\beta)\in P} \tanh K_{\alpha\beta}. \tag{4}$$

Here, $\mathbb{P}$ is the set of all polygons on the graph G; a set of edges P in G is called a polygon on G if each point in G is incident to an even number of edges in P. A few remarks are in order: (i) the empty set is a polygon; (ii) a subgraph $G(P)$ generated by a polygon P is not necesarily connected; (iii) every connected component of $G(P)$ has a closed Euler trail (i.e., can be *drawn with one stroke along a closed path*) for any polygon P. For example



is a polygon (thick lines) on a graph (dashed lines; this graph is called a square lattice). We can interpret the summation in eq. (4) as a weighted summation over all polygons on G with weight $\tanh K_{\alpha\beta}$ on each edge (α, β).

Now consider the average

$$\langle \log Z(\mathbf{K}) \rangle_{\mathbf{K}} = N \log 2 + M \log\cosh K + \Big\langle \log \Big(\sum_{P\in\mathbb{P}} \prod_{(\alpha,\beta)\in P} \tanh K_{\alpha\beta} \Big) \Big\rangle_{\mathbf{K}}.$$

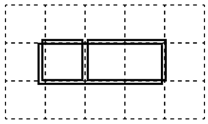
To evaluate the last term we employ the replica trick. Thus we are to calculate

$$\Big\langle \Big(\sum_{P\in\mathbb{P}} \prod_{(\alpha,\beta)\in P} \tanh K_{\alpha\beta} \Big)^n \Big\rangle_{\mathbf{K}} \tag{5}$$

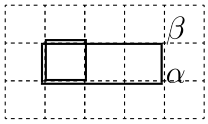
for positive integers n. Expand $(\cdots)^n$ in (5); then each term represents a product of weights for n species (or n copies; n replicas) of polygons, each of which came from each factor in $(\cdots)^n$. We shall call such a figure, corresponding to each term, consisting of polygons of n species an n-ply polygon. Finally we must average this series. Since

$$\langle (\tanh K_{\alpha\beta})^k \rangle_{\mathbf{K}} = \begin{cases} (\tanh K)^k & \text{if } k \text{ is even,} \\ 0 & \text{if } k \text{ is odd} \end{cases}$$

only terms that have an even number of edges of polygons of n species on each edge of G remain non-zero, and the weight of each term is averaged to $(\tanh K)^k$ where k is the number of edges of polygons of the term. For example, if G is a square lattice, the term corresponding to the diagram



consisting of three polygons of different species contributes to (5) with weight $(\tanh K)^{18}$ since a total of 18 edges of the polygons are there; on the other hand the term corresponding to



vanishes in (5) since, say, the edge (α, β) is occupied by a single polygon.

Thus, we can rewrite (5) as

$$\sum_{\text{allowed } \tilde{P} \in \tilde{\mathbb{P}}_n} \Big(\tanh K \Big)^{\# \tilde{P}} \tag{6}$$

where $\tilde{\mathbb{P}}_n$ is the set of all n-ply polygons, an *allowed* n-ply polygon means that every edge in G is occupied by an even number of edges of the n-ply polygon, and $\#\tilde{P}$ means the number of edges of the n-ply polygon $\tilde{P}$.

4. Reformulation based on the low-temperature expansion

Our second reformulation of (2) is based on the so-called low-temperature expansion. Let us rewrite (1) as

$$Z(\mathbf{K}) = e^{\sum_{(\alpha,\beta)\in B} K_{\alpha\beta}} \sum_{\sigma \in \mathbb{C}} \prod_{(\alpha,\beta)\in B} x_{\alpha\beta}^{\frac{1-\sigma_\alpha \sigma_\beta}{2}}$$

where $x_{\alpha\beta} = e^{-2K_{\alpha\beta}}$. If we decompose the set of all spin configurations as $\mathbb{C} = \mathbb{C}^+ \cup \mathbb{C}^-$ (disjoint union) where $\mathbb{C}^+ = \{1\} \times \{-1, 1\}^{N-1}$, then

$$Z(\mathbf{K}) = 2e^{\sum_{(\alpha,\beta)\in B} K_{\alpha\beta}} \sum_{\sigma \in \mathbb{C}^+} \prod_{(\alpha,\beta)\in B} x_{\alpha\beta}^{\frac{1-\sigma_\alpha \sigma_\beta}{2}}. \tag{7}$$

This expression can be interpreted graphically. In the rest of this section we assume that the graph G is embeddable into a 2-surface. Thus, 2-cells (cell for short) of G surrounded by edges are well-defined, and we can consider the dual of G. The dual graph G^* of G is defined as follows: place a point on each cell of G, and let V^* be the set of all such points; for each edge $e \in B$ connect two points in V^* placed on cells adjacent to this edge e by an edge e^* which goes across e, and let B^* be the set of all such edges; then G^* is the pair of V^* and B^*. Note that a point, an edge, and a cell in G^* correspond to a cell, an edge, and a point in G, respectively; and especially that an edge in G^* can be specified uniquely by the corresponding edge in G. Now consider a polygon on the dual graph G^* and look at (7). Since

$$\frac{1-\sigma_\alpha\sigma_\beta}{2} = \begin{cases} 1 & \text{if } (\sigma_\alpha, \sigma_\beta) = (-1,1), (1,-1), \\ 0 & \text{if } (\sigma_\alpha, \sigma_\beta) = (-1,-1), (1,1), \end{cases}$$

we notice that there exists a one-to-one correspondence between $\mathbb{C}^+$ and the set $\mathbb{P}^*$ of all polygons on G^*. Thus we get

$$Z(\mathbf{K}) = 2e^{\sum_{(\alpha,\beta)\in B} K_{\alpha\beta}} \sum_{P^*\in\mathbb{P}^*} \prod_{(\alpha,\beta)\in P^*} x_{\alpha\beta}. \tag{8}$$

To calculate the average of log of (8), we again use the replica trick. So our task is to evaluate

$$\Big\langle \big(\sum_{P^*\in\mathbb{P}^*} \prod_{(\alpha,\beta)\in P^*} x_{\alpha\beta} \big)^n \Big\rangle_{\mathbf{K}} \tag{9}$$

for positive integers n. Since

$$\langle x_{\alpha\beta}^k \rangle_{\mathbf{K}} = \cosh(2kK) \qquad \text{for } k = 0, 1, 2, \ldots$$

we can rewrite (9) as

$$\sum_{\tilde{P}^*\in\tilde{\mathbb{P}}_n^*} \prod_{(\alpha,\beta)\in B^*} \cosh\big(2\nu_{\alpha\beta}(\tilde{P}^*)K\big) \tag{10}$$

where $\tilde{\mathbb{P}}_n^*$ is the set of all n-ply polygons on G^*, and $\nu_{\alpha\beta}(\tilde{P}^*)$ is the number of edges in the n-ply polygon $\tilde{P}^*$ occupying the edge $(\alpha,\beta) \in B^*$.

5. Example

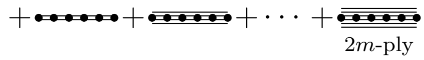
To demonstrate how our reformulations work, we give explicit calculations for the cyclic chain G of N points. Note that in this case the direct computation (without using the replica trick) is possible: since $\sum_{\sigma\in\mathbb{C}} \prod_{(\alpha,\beta)\in B} \big(1+\sigma_\alpha\sigma_\beta z_{\alpha\beta}\big) = 2^N\big(1+\prod_{(\alpha,\beta)\in B} z_{\alpha\beta}\big)$, where $z_{\alpha\beta} = \tanh K_{\alpha\beta}$, and

$$\begin{aligned} \Big\langle \log\big(1+\prod_{(\alpha,\beta)\in B} z_{\alpha\beta}\big) \Big\rangle_{\mathbf{K}} &= \Big\langle \sum_{n=1}^{\infty} (-1)^{n-1}\frac{1}{n} \big(\prod_{(\alpha,\beta)\in B} z_{\alpha\beta} \big)^n \Big\rangle_{\mathbf{K}} \\ &= -\sum_{m=1}^{\infty} \frac{1}{2m} z^{2mN} = \frac{1}{2}\log\big(1-z^{2N}\big) \end{aligned}$$

where $z = \tanh K$, we have from eq.(3)

$$\langle \log Z(\mathbf{K}) \rangle_{\mathbf{K}} = N\log 2 + N\log\cosh K + \frac{1}{2}\log\big(1-z^{2N}\big). \tag{11}$$

5.1. **The high-temperature expansion.** Let us denote $\sum\prod \tanh K_{\alpha\beta}$ in (5) by S, and $\langle\cdots\rangle_{\mathbf{K}}$ by $\langle\cdots\rangle$. Since there are only two polygons (the empty and the all edges) on the cyclic chain, the computaion is straightforward. Graphically

$\langle S^{2m}\rangle = \mathbf{1}$ 

It gives $\langle S^{2m}\rangle = 1 + \binom{2m}{2}z^{2N} + \binom{2m}{4}z^{4N} + \cdots + \binom{2m}{2m}z^{2mN} = \frac{1}{2}\{(1+z^N)^{2m} + (1-z^N)^{2m}\}$. Similar expression is obtained for $\langle S^{2m+1}\rangle$, and we get $\langle S^n\rangle = \frac{1}{2}\{(1+z^N)^n + (1-z^N)^n\}$ for all n. Hence

$$\lim_{n\to 0}\frac{\partial}{\partial n}\langle S^n\rangle = \frac{1}{2}\{\log(1+z^N) + \log(1-z^N)\} = \frac{1}{2}\log(1-z^{2N})$$

which gives eq.(11) as expected.

5.2. **The low-temperature expansion.** The dual graph G^* consists of two points and N edges. Since the number of polygons on G^* is $\binom{N}{0} + \binom{N}{2} + \binom{N}{4} + \ldots + \binom{N}{2[N/2]} = 2^{N-1}$ the computation should become more elaborate. We could not succeed in reproducing eq.(11); but we show the temporary computaions here. Let us denote $\sum\prod x_{\alpha\beta}$ in (9) by S. Then, $\langle S\rangle = \sum_{i=0}^{[N/2]}\binom{N}{2i}(\cosh 2K)^{2i}$ and, inductively, if

$$\langle S^{n-1}\rangle = \sum_{k_1=0}^{[N/2]}\cdots\sum_{k_{n-1}=0}^{[N/2]} A^{(n-1)}_{k_{n-1},\dots,k_1} c_{n-1}^{k_{n-1}}\cdots c_1^{k_1}$$

where $c_m = \cosh(2mK)$, then

$$\begin{aligned}\langle S^n\rangle = &\sum_{k_1=0}^{[N/2]}\cdots\sum_{k_{n-1}=0}^{[N/2]} A^{(n-1)}_{k_{n-1},\dots,k_1} c_{n-1}^{k_{n-1}}\cdots c_1^{k_1}\\ &\cdot\sum_{i=0}^{[N/2]}\underbrace{\sum\cdots\sum}_{\substack{0\le p_1,\dots,p_n\le 2i\\ p_1+\ldots+p_n=2i}}\binom{k_{n-1}}{p_n}\binom{k_{n-2}}{p_{n-1}}\cdots\binom{k_1}{p_2}\binom{N-k_1-\ldots-k_{n-1}}{p_1}\\ &\cdot\Big(\frac{c_n}{c_{n-1}}\Big)^{p_n}\Big(\frac{c_{n-1}}{c_{n-2}}\Big)^{p_{n-1}}\cdots\Big(\frac{c_2}{c_1}\Big)^{p_2}\Big(\frac{c_1}{c_0}\Big)^{p_1}.\end{aligned}$$

For $n=1,2$, explicit expressions can be obtained: $\langle S\rangle = \frac{1}{2}\{(1+c_1)^N + (1-c_1)^N\}$ and

$$\begin{aligned}\langle S^2\rangle &= \underbrace{\sum\sum\sum}_{\substack{0\le k_1,k_2,k_3\le N,\,k_1+k_2+k_3\le N\\ k_1,k_2,k_3\text{ have the same parity}}}\binom{N}{k_1,k_2,k_3,N-k_1-k_2-k_3}(c_2)^{k_1}(c_1)^{k_2+k_3}\\ &= \frac{1}{4}\{(1+2c_1+c_2)^N + (1-2c_1+c_2)^N + 2(1-c_2)^N\}.\end{aligned}$$

For larger n we have not succeeded in finding such explicit forms.

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