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Bounds on Ising partition functions II: Application to frustration

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Abstract. Applying the method developed in I, two families of Ising models, one on the Kagomé lattice and the other on the square lattice, are studied. The interactions are chosen so that the models are strongly frustrated. It is shown that the free energy is analytic at every positive temperature. For the Kagomé lattice models, the correlations in the totally symmetric equilibrium state are analytic for $T > 0$ and decay exponentially at every temperature, including $T = 0$.

1. Introduction

In the first paper (I) of this series we developed a method for locating the zeroes of Ising partition functions. Now we apply this method to study the analyticity properties of the free energy and the correlations in certain frustration models. In these systems a competition occurs among the interactions which may prevent the spins to take up fixed orientations in the ground state. This property is easy to see on small systems containing a few number of competing interactions: the correlation functions may remain smaller than unity even at $T = 0$. We will make use of this fact in the following way. Considering some special models, the whole set of bonds will be divided into small subsets (each containing 3 or 4 bonds, in our examples) so that frustration occurs in any subset. Using the results of I, we obtain a high temperature (H.T.) expansion for the free energy and the correlations in which the 'small variables' are the correlations on the frustrated small subsets instead of the usual quantities, $\tanh \beta J_b$. Knowing that the formers do not increase up to unity while the latters do that with β going to infinity, one may expect a better convergence for our modified H.T. series than for the conventional one.

In this paper we consider examples where the convergence and, therefore, the domain of analyticity extends over the whole positive temperature axis. A prototype of the models for which the best results can be obtained is a family of frustration models on the Kagomé lattice, discussed in Section 2. Beside the analyticity of the free energy for any positive temperature T , we can prove that the correlations in the totally symmetric equilibrium state (i.e., the state corresponding to vacuum boundary conditions) are analytic for any $T > 0$ and they decay exponentially at every temperature, including $T = 0$. This latter property is

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very peculiar and the author does not know about other classical models with a similar behaviour. In Section 3, we study a similar family of models on the square lattice. These are interesting as marginal cases in which the absence of phase transitions can be proved with our method: one can show that the free energy is analytic at any $T > 0$ but no result, similar to that valid for the Kagomé lattice, is obtained for the correlations.

The notations applied in this paper are those introduced in I. We will refer to the formulas of the first paper as I.1 etc.

The lengthy proof of the exponential clustering on the Kagomé lattice is relegated to an Appendix.

2. Frustration models on the Kagomé lattice

The Kagomé lattice is a plane lattice built up from regular triangles and hexagons so that every edge is shared by two different types of polygons. Therefore, if $J_b \neq 0$ only for nearest neighbour pairs (nnp), their set B can be covered with the set $\{B^i\}$ of pairwise disjoint triangles:

$$B^i = (b^1, b^2, b^3)$$

where b^k are nnp forming a triangle (Fig. 1). The elements of the H.T. Group can be visualised as graphs of even order, and the members of $\text{inf } G$ are the simple (non-crossing) polygons. Now $\text{inf } G$ does not generate G uniquely because crossing graphs have more than one decomposition. It is easy to see, however, that $\{B^i\}$ may play the role of the cover $\{Q^i\}$ of Lemma 2: if G^0 is the subgroup associated with the cover $\{B^i = Q^i\}$ via equation I.9 then G/G^0 is uniquely

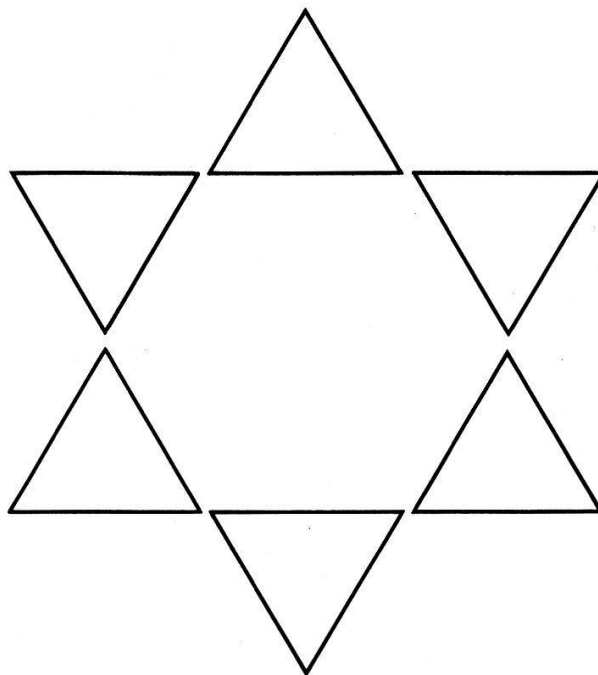


Figure 1

The bonds of the Kagome lattice and their covering with the set of triangles. The three bonds of any triangle form an element of $\text{inf } G$ and, also, of G^0 . A general element of G^0 is a set of triangles. The six edges of a hexagon form an element of $\text{inf } G$ and they represent an element of $\text{inf } G/G^0$ as well.

generated by $\inf G/G^0$. (This is true because every lattice site belongs to only two triangles and for any $A \in G/G^0$, s_A has at most one element common with $P(B^i)/G^i$.) Let us consider now G^i and the cosets of $P(B^i)$ according to G^i . The corresponding quotient group is

$$P(B^i)/G^i = \{G^i, a^1, a^2, a^3\}$$

where

$$G^i = \{\emptyset, \{b^1, b^2, b^3\}\}$$

and

$$a^k = \{b^k, \{b^l, b^m\}\}$$

with $(k, l, m) = (1, 2, 3)$ and its cyclic permutations. The coset a^k can be indexed with the nnp b^k ; the variable, assigned to a^k through equation I.17c, is

$$\zeta_{b^k} = (z_{b^k} + z_{b^l}z_{b^m}) / (1 + z_{b^k}z_{b^l}z_{b^m}) \tag{1}$$

where z_b are given by equation I.30. According to I.31, for real non-negative values of β , ζ_{b^k} is a pair correlation function belonging to the nnp b^k . It is useful to introduce the variable w_b

$$w_b \equiv \tanh |J_b| \beta \tag{2}$$

Then (1) becomes

$$\zeta_{b^k} = \text{sgn } J_b (w_{b^k} + p(i)w_{b^l}w_{b^m}) / (1 + p(i)w_{b^k}w_{b^l}w_{b^m})$$

where

$$p(i) = \prod_{b \in B^i} \text{sgn } J_b \tag{3}$$

Let us notice that (3) simplifies to

$$\zeta_b = (\text{sgn } J_b) w_i / (1 - p(i)w_i + w_i^2) \tag{4}$$

if $w_b = w_i$ for all $b \in B^i$. This can be reached by choosing $|J_b|$ to be the same for all nnp in a given triangle.

Let now

$$B = \bigcup_{i=1}^N B^i$$

and consider the function

$$\psi(\beta) = \lim_{N \rightarrow \infty} \psi_N(\beta) \tag{5a}$$

with

$$\begin{aligned} \psi_N(\beta) &= (1/N) \log [R(\beta)/R^0(\beta)] \\ &= (1/N) \sum_{i=1}^{N-1} \log (1 + t_{[i]}^{i+1}(\beta)) \end{aligned} \tag{5b}$$

Here R is defined by I.29, R^0 corresponds to I.13:

$$R^0(\beta) = \prod_{i=1}^N \left(1 + p(i) \prod_{b \in B^i} w_b(\beta) \right) \quad (6)$$

and $t_{[i]}^{i+1}(\beta)$ is determined by R and R^0 through equations I.17–I.20 and I.30. Apart from a term analytic in β for $\beta \in [0, \infty)$, $\psi(\beta)$ is the specific free energy of the system; we know the existence of the limit (5a) for real β if the potential is periodic. Notice that $\psi(\beta)$ depends on β only through ζ_b . We have the following result.

Theorem 1. Consider a periodic nnp potential on the Kagomé lattice which satisfies the condition that for any triangle B^i

$$|J_b| = |J_{b'}| \quad \text{for } b, b' \in B^i. \quad (7a)$$

Then

(i) $\psi(\beta)$ is an analytic function inside the domain

$$\mathcal{D} = \{\beta \in \mathbb{C} : |\zeta_b(\beta)| < 0.34 \text{ for all nnp } b\}$$

(ii) the limit

$$\lim_{N \rightarrow \infty} \langle \sigma^d \rangle_B = \langle \sigma^d \rangle \quad (8)$$

exists and is an analytic function of β inside \mathcal{D} , for any finite subset d of the lattice; moreover,

$$|\langle \sigma^{d_1} \sigma^{d_2} \rangle - \langle \sigma^{d_1} \rangle \langle \sigma^{d_2} \rangle| \leq 10^6 e^{-0.09\rho(d_1, d_2)} \quad (9)$$

holds in \mathcal{D} ($\rho(d_1, d_2)$ is the distance between d_1 and d_2).

Remarks. 1. The theorem refers to a family of potentials. Apart from the freedom in choosing $|J_b|$ to be different in different triangles one can choose the signs $p(i)$ and

$$q(k) = \text{sgn} \prod_{b \in k \text{th hexagon}} J_b$$

independently. This is a general property of two dimensional lattices.

2. Let us consider the case when

$$p(i) = -1 \quad \text{for all } B^i. \quad (7b)$$

From (4) and (7a,b) it follows that $|\zeta_b| \leq \frac{1}{3}$ for any real β . As a consequence, $\psi(\beta)$ and the correlations in the totally symmetric equilibrium state are analytic at any real non-negative β and the correlations decay exponentially at any $\beta \geq 0$, including $\beta = +\infty$.

It is easy to check that to any potential satisfying (7a,b) there exist infinitely many periodic ground states. The simplest example is the antiferromagnet, $J_b = -1$ for all nnp; this corresponds to $q(k) \equiv 1$. The plot of the domain

$$|w/(1+w+w^2)| < 0.34,$$

relevant in the case (7b), is shown on Fig. 2.

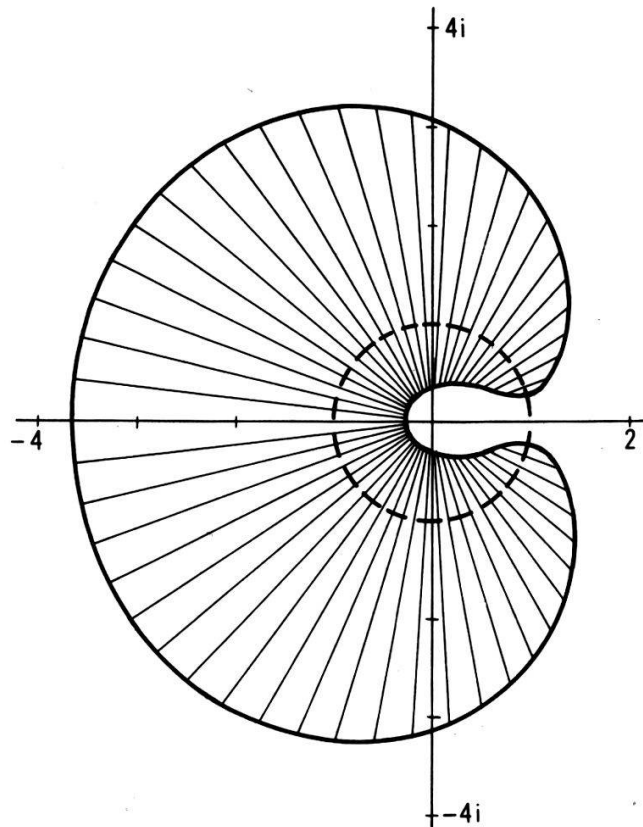


Figure 2

The domain of analyticity (outside the shaded region) on the complex $\tanh |J_b| \beta$ plane, for the Kagomé lattice models.

Proof. (i) A brief inspection may convince us that for N_n of equation I.15 the following values can be chosen:

$$\begin{aligned}
 N_n &= 0 && \text{for } n \text{ is odd and } n = 2, 4, 8 \\
 N_6 &= 3, && N_{10} = 15, \quad N_{12} = 6 \\
 N_{2n} &= 2^n && \text{for } n \geq 7.
 \end{aligned}$$

Putting these values and $x = 0.34$, $\varepsilon = 0.1$ into I.2 one finds that the inequality is satisfied. The statement is then a consequence of the uniform boundedness of $\{\psi_N(\beta)\}$ in \mathcal{D} and Vitali's convergence theorem.

(ii) The existence and analyticity of the correlations $\langle \sigma^d \rangle$ follow from the uniform boundedness of $\langle \sigma^d \rangle_B$ in the domain \mathcal{D} and from the H.T. existence of the limit (8). The former is a consequence of I.27 and the estimate

$$N_n^d \leq 2^n \tag{10}$$

which is valid for any $d \subset \mathbb{Z}$.

If $|d|$ (the number of points in d) is odd, the correlations vanish identically. If $|d_1|$ and $|d_2|$ are odd numbers then

$$|\langle \sigma^{d_1 \cup d_2} \rangle| \leq 4.1 e^{-0.27\rho(d_1, d_2)}$$

follows immediately from I.27 and (10) and the fact that

$$N_n^{d_1 \cup d_2} = 0$$

for $n < \rho(d_1, d_2)$.

For $|d_1|$ and $|d_2|$ even, the weaker bound (9) can be obtained. The proof is lengthy and we leave it to the Appendix.

4. Frustration models on the square lattice

Again, we confine ourselves to nnp potentials. Consider the squares of \mathbf{Z}^2 forming an infinite chessboard and let B^i be the set of the four nnp bordering the i th black square:

$$B^i = \{b^1, \dots, b^4\}.$$

Now $\cup B^i$ covers the whole set of nnp (Fig. 3). Due to the crossing graphs, $\text{inf } G$ does not generate G uniquely while G/G^0 (where G^0 is defined by I.9) is uniquely generated by $\text{inf } G/G^0$. Using the variables introduced in (2) and (3) we find

$$\xi_{b^1} = \text{sgn } J_{b^1} \left(w_{b^1} + p(i) \prod_{j=2}^4 w_{b^j} \right) / \left(1 + p(i) \prod_{b \in B^i} w_b \right)$$

and

$$\zeta_c = (\text{sgn } J_{b^1} J_{b^2}) (w_{b^1} w_{b^2} + p(i) w_{b^3} w_{b^4}) / \left(1 + p(i) \prod_{b \in B^i} w_b \right)$$

where c is a diagonal pair or it is the set of the four sites of B^i . If $w_b = w_i$ for all $b \in B^i$ and $p(i) = -1$ then ζ_c vanishes and

$$\zeta_b = (\text{sgn } J_b) w_i / (1 + w_i^2) \equiv (\text{sgn } J_b) \xi_i. \tag{11}$$

Let $\psi(\beta)$ be defined for the present group G and cover B , by equations (5) and (6). We obtain the following theorem for $\psi(\beta)$.

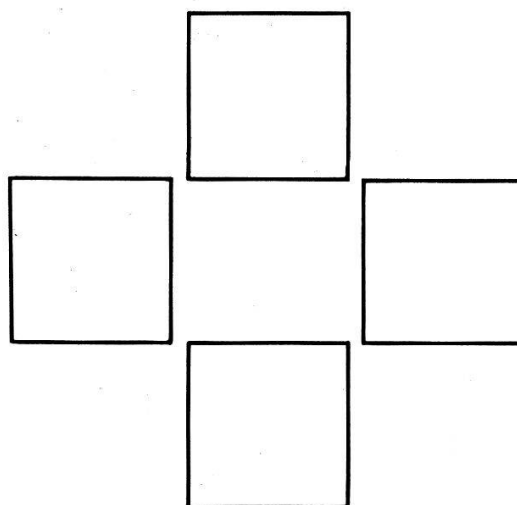


Figure 3

The bonds of the square lattice and their covering with the set of ‘black’ squares. The four bonds of any black square form an element of $\text{inf } G$ and, also, of G^0 . A general element of G^0 is a set of black squares. The four edges of a ‘white’ square form an element of $\text{inf } G$ and they represent an element of $\text{inf } G/G^0$ as well.

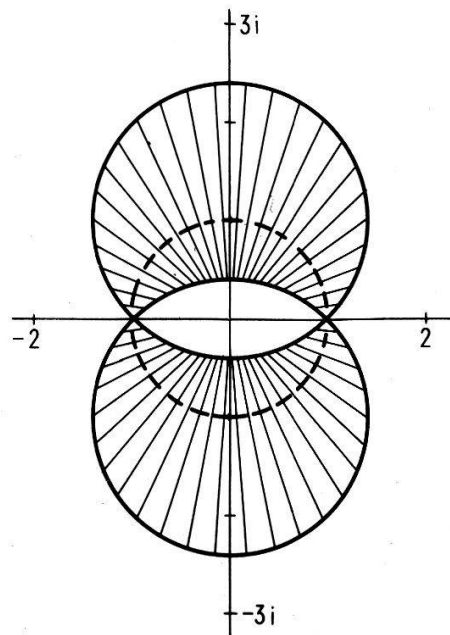


Figure 4

The domain of analyticity (outside the shaded region) on the complex $\tanh |J_b| \beta$ plane, for the square lattice models.

Theorem 2. Consider a periodic nnp potential on the square lattice which satisfies the conditions (7a,b). Then $\psi(\beta)$ is an analytic function inside the domain

$$\mathcal{D}_{sq} = \{\beta \in \mathbb{C} : |\zeta_b| < \frac{1}{2} \text{ for all } b\}.$$

Remarks. 1. The theorem refers to a family of potentials. $|J_b|$ may vary from square to square and the signs

$$q(k) = \text{sgn} \prod_{b \in k\text{th white square}} J_b$$

can be chosen independently. For periodic potentials satisfying (7) there are infinitely many periodic ground states. The simplest examples can be obtained by fixing $|J_b| = 1$ and choosing either $q(k) \equiv -1$ or $q(k) \equiv 1$. These give the so called ‘odd’ and ‘chessboard’ models, respectively, whose free energies were calculated exactly and found to be analytic for any positive temperature ([1], [2]).

2. The analyticity of $\psi(\beta)$ follows for any real finite β . The domain $|w/(1+w^2)| < \frac{1}{2}$ is shown on Fig. 4. We cannot prove the analyticity and clustering of the correlations for all $\beta \in [0, \infty)$, the reason of which becomes obvious from the proof of the theorem. However, these properties could be shown, with the method applied for the Kagomé lattice, in a relatively large H.T. domain.

Proof. Asymptotically, $N_n = 2^n$ is an upper bound for $N_n(i)$ and one would find difficult to improve it. On the other hand, as (11) shows, $|\zeta_b| = \frac{1}{2}$ if $1/\beta = 0$. One should choose $x = \frac{1}{2}$ in equation I.2 in order to obtain analyticity for all $\beta \in [0, \infty)$. However, with these N_n and x the inequality I.2 cannot be satisfied for any $\varepsilon < 1$.

We need to use some special properties of the lattice and the potential. Let us

rewrite the formula I.18 for $t_\alpha^i, i \notin \alpha$:

$$t_\alpha^i = \sum_{b \in B^i} \zeta_b \sum_{s \in S_\alpha^b} \zeta^s / T_\alpha = \sum_{b \in B^i} \zeta_b T_\alpha^b / T_\alpha$$

$$S_\alpha^b = \left\{ s \subset \bigcup_{j \in \alpha} B^j : |s \cap B^j| \leq 1 \text{ and } \prod_{b' \in s} b' = b \right\}. \tag{12}$$

Now t_α^i depends on β through the set of variables $\xi = \{\xi_k = (\text{sgn } J_b) \zeta_b\}_{k=1,2,\dots}$, each belonging to a square B^k .

Below we show that, with a suitable choice for the numbering of the set $\{B^i\}$, one can obtain the bound

$$|t_{[i]}^{i+1}(\xi)| \leq \frac{1}{2}$$

for all i , if $|\xi_k| \leq \frac{1}{2}$ for all k .

(i) If $0 \leq \xi_k \leq \frac{1}{2}$ for all k then it is possible to define a potential and some $\beta \geq 0$ so that they determine just these ξ_k through equations (2) and (11). As a consequence, T_α^b / T_α is a correlation and

$$t_\alpha^i(\xi) = \sum_{b \in B^i} \zeta_b \langle \sigma^b \rangle_{B_\alpha}$$

where

$$B_\alpha = \bigcup_{j \in \alpha} B^j.$$

Now if $n(i, \alpha)$ is the number of those vertices which are shared between B^i and the squares of B_α then

$$|t_\alpha^i(\xi)| \leq \begin{cases} 1 & \text{if } n(i, \alpha) \leq 3 \\ \frac{1}{2} & \text{if } n(i, \alpha) \leq 2 \end{cases} \tag{13}$$

because $S_\alpha^b \neq \emptyset$ for at most two or one $b \in B^i$, respectively.

(ii) Let

$$\tilde{t}_\alpha^i(\xi) = \sum_{\substack{s \in S_{\alpha \cup \{i\}} \\ i \in s}} \prod_{b \in s} e_b \prod_{j \in s} \xi_j / \sum_{s \in S_\alpha} \prod_{b \in s} e_b \prod_{j \in s} \xi_j$$

where e_b is defined for each nnp so that

$$e_b = \begin{cases} -1 & \text{if } b \text{ is the lower nnp of some } B^i \\ 1 & \text{otherwise} \end{cases}$$

Clearly, \tilde{t}_α^i is a function of the form of I.18 or (12): it corresponds to a particular choice for the signs of the interactions. One can show by elementary methods that

$$\prod_{b \in s} e_b = -1$$

for all $s \in \text{inf } S$. Now let $0 \leq \xi_k \leq \frac{1}{2}$ for all k , then

$$\tilde{t}_\alpha^i(\xi) \leq 0 \tag{14}$$

for all α and $i \notin \alpha$. Indeed,

$$\tilde{t}_\alpha^i(\xi) = - \sum_{\substack{s \in \text{inf } S_\alpha \cup \{i\} \\ i \in s}} \prod_{j \in s} \xi_j / \prod_{k=2}^{|\xi|} (1 + \tilde{t}_{\alpha-s'k}^{j_k}(\xi)). \tag{15}$$

Now

$$s = \{i, j_2, \dots, j_n\}$$

is a set of indices of squares which form a ring by joining via vertices. The numbering can be chosen so that neighbouring indices belong to joining squares. Therefore,

$$n(j_k, \alpha - s'k) = n(j_k, \alpha - \{j_2, \dots, j_n\}) \leq 3$$

which implies

$$|\tilde{t}_{\alpha-s'k}^{j_k}(\xi)| \leq 1 \tag{16}$$

by equation (13). Equations (15) and (16) then prove (14).

(iii) Let $|\xi|$ denote the set $\{|\xi_k|\}_{k=1,2,\dots}$. Suppose that $|\xi_k| \leq \frac{1}{2}$ for all k . Then

$$|t_\alpha^i(\xi)| \leq -\tilde{t}_\alpha^i(|\xi|) \tag{17}$$

This can be shown by induction. For, $t_\alpha^i = 0$ if $|\alpha| < 3$; if $\alpha = \{1, 2, 3\}$ and B^1, \dots, B^4 surround a white square then

$$|t_{\{1,2,3\}}^4| = |\xi_1| \cdot |\xi_2| \cdot |\xi_3| \cdot |\xi_4| = -\tilde{t}_{\{1,2,3\}}^4(|\xi|).$$

In the n th step,

$$\begin{aligned} |t_\alpha^i(\xi)| &\leq \sum_{\substack{s \in \text{inf } S_\alpha \cup \{i\} \\ i \in s}} \prod_{j \in s} |\xi_j| / \prod_{k=2}^{|\xi|} |1 - t_{\alpha-s'k}^{j_k}(\xi)| \\ &\leq \sum_{\substack{s \in \text{inf } S_\alpha \cup \{i\} \\ i \in s}} \prod_{j \in s} |\xi_j| / \prod_{k=2}^{|\xi|} |1 + \tilde{t}_{\alpha-s'k}^{j_k}(|\xi|)| \\ &= -\tilde{t}_\alpha^i(|\xi|) \end{aligned}$$

Here we applied the induction together with (16).

(iv) Consider now the set $\{B^1, B^2, \dots\}$ which covers all nnp of the lattice. Let the numbering be chosen so that B^i joins B^{i+1} through a vertex and the whole set forms an infinite spiral of squares. Then

$$n(i+1, [i]) \leq 2$$

and (13) implies that

$$-\tilde{t}_{[i]}^{i+1}(|\xi|) \leq \frac{1}{2}.$$

This, together with (17) proves that

$$|t_{[i]}^{i+1}(\xi)| \leq \frac{1}{2} \tag{18}$$

for all i . The remaining is an application of Vitali's theorem.

Appendix. Exponential clustering

Let $d_1, d_2 \subset \wedge$ be disjoint sets with even number of points. Now we have to estimate

$$\langle \sigma^{d_1} \sigma^{d_2} \rangle_B - \langle \sigma^{d_1} \rangle_B \langle \sigma^{d_2} \rangle_B = (T^{d_1 \cup d_2} T - T^{d_1} T^{d_2}) / T^2. \quad (\text{A.1})$$

This can be done by dividing (A.1) into terms and estimating them distinctly.

$$T^{d_1 \cup d_2} = \sum_{s \in \inf S^{d_1 \cup d_2}} \zeta^s T_{[N]-s} = T_1 + T_2$$

where

$$T_1 = \sum_{\substack{s_1 \in \inf S^{d_1} \\ s_1 \cap s_2 = \emptyset}} \sum_{s_2 \in \inf S^{d_2}} \zeta^{s_1} \zeta^{s_2} T_{[N]-s_1-s_2}$$

and

$$T_2 = \sum'_{s \in \inf S^{d_1 \cup d_2}} \zeta^s T_{[N]-s}$$

the prime indicating that no part of s is an element of $\inf S^{d_1}$. If s occurs in the summation for T_2 then $|s| \geq \rho$, the distance of d_1 and d_2 , and

$$|T_2/T| \leq \sum_{n \geq \rho} (2x/(1-\varepsilon))^n = (1-y)^{-1} y^\rho. \quad (\text{A.2})$$

Here we used the bound (10) and

$$\begin{aligned} |\zeta^s| &\leq x^{|s|} \\ |t_\alpha^i| &\leq \varepsilon \\ y &= 2x/(1-\varepsilon). \end{aligned} \quad (\text{A.3})$$

On the other hand,

$$T^{d_1} T^{d_2} = U_1 + U_2$$

where

$$U_1 = \sum_{\substack{s_1 \in \inf S^{d_1} \\ s_2 \in \inf S^{d_2} \\ s_1 \cap s_2 = \emptyset}} \zeta^{s_1} \zeta^{s_2} T_{[N]-s_1} T_{[N]-s_2}$$

and

$$U_2 = \sum_{\substack{s_1 \in \inf S^{d_1} \\ s_2 \in \inf S^{d_2} \\ s_1 \cap s_2 \neq \emptyset}} \zeta^{s_1} \zeta^{s_2} T_{[N]-s_1} T_{[N]-s_2}.$$

Now if (s_1, s_2) occurs in the summation for U_2 then $|s_1| + |s_2| \geq \rho$. We can use the simple estimate

$$\text{card} \{(s_1, s_2) \in \inf S^{d_1} \times \inf S^{d_2} : |s_1| + |s_2| = n\} \leq n 2^n \quad (\text{A.4})$$

to obtain the bound

$$|U_2/T^2| \leq \sum_{n \geq \rho} ny^n \leq (1-y)^{-2} \rho y^\rho. \tag{A.5}$$

Let us consider $TT_1 - U_1$.

$$TT_1 - U_1 = \sum_{\substack{s_1 \in \inf S^{d_1} \\ s_1 \cap s_2 = \emptyset}} \sum_{s_2 \in \inf S^{d_2}} \zeta^{s_1} \zeta^{s_2} (T_{[N]} T_{[N]-s_1-s_2} - T_{[N]-s_1} T_{[N]-s_2}) = \sum'_{(s_1, s_2)} \zeta^{s_1} \zeta^{s_2} \Delta(s_1, s_2) \tag{A.6}$$

where $T_{[N]} = T$. Writing up the difference in the parentheses explicitly, one can see that many terms cancel out. Omitting a lengthy intermediate speculation, we present the surviving terms:

$$\begin{aligned} \Delta(s_1, s_2) = & \sum_{v \in V_0} \left(\prod_{s \in v} \zeta^s \right) T_{[N]-s_1-s_2-v} T_{[N]-s_1-s_2} \\ & - \sum_{(v_1, v_2) \in V_{12}} \prod_{i=1}^2 \left(\prod_{s \in v_i} \zeta^s \right) T_{[N]-s_1-s_2-v_1} T_{[N]-s_1-s_2-v_2} \\ & + \sum_{(v_1, v_2, v_3) \in V_{123}} \prod_{i=1}^3 \left(\prod_{s \in v_i} \zeta^s \right) T_{[N]-s_1-s_2-v_1-v_2} T_{[N]-s_1-s_2-v_3}. \end{aligned} \tag{A.7}$$

With the definition

$$[S] = \{ \{s'_1, \dots, s'_k\} \subset \inf S : s'_i \cap s'_j = \emptyset \text{ for } i \neq j \},$$

the sets V_0, V_{12}, V_{123} are given as follows:

$$\begin{aligned} V_0 = & \{ \{s'_1, \dots, s'_k\} \in [S] : s'_i \cap (s_1 \cup s_2) \neq \emptyset \text{ for } i = 1, \dots, k \\ & \text{and } s'_j \cap s_1 \neq \emptyset, s'_j \cap s_2 \neq \emptyset \text{ for some } 1 \leq j \leq k \} \\ V_1 = & \{ \{s'_1, \dots, s'_k\} \in [S_{[N]-s_2}] : s'_i \cap s_1 \neq \emptyset \text{ for } i = 1, \dots, k \} \\ V_2 = & \{ \{s'_1, \dots, s'_k\} \in [S_{[N]-s_1}] : s'_i \cap s_2 \neq \emptyset \text{ for } i = 1, \dots, k \} \\ V_{12} = & \{ (v_1, v_2) \in V_1 \times V_2 : v_1 \cap v_2 \neq \emptyset \} \end{aligned}$$

where

$$\begin{aligned} \mathbf{v} = & \bigcup_{s \in v} \mathbf{s}; \\ V_{123} = & \{ (v_1, v_2, v_3) \in V_1 \times V_2 \times [S_{[N]-s_1-s_2}] : (v_1, v_2) \in (V_1 \times V_2) - V_{12} \\ & \text{and } \mathbf{s} \cap (\mathbf{v}_1 \cup \mathbf{v}_2) \neq \emptyset \text{ for any } s \in v_3 \\ & \text{and } \mathbf{s} \cap \mathbf{v}_1 \neq \emptyset, \mathbf{s} \cap \mathbf{v}_2 \neq \emptyset \text{ for some } s \in v_3 \}. \end{aligned}$$

Dividing (A.7) by T^2 and applying (A.3) we find

$$|\Delta(s_1, s_2)/T^2| \leq (1-\varepsilon)^{-2|s_1|-2|s_2|} \sum_{v \in V_0 \cup V_{12} \cup V_{123}} (y/2)^{|v|} \tag{A.8}$$

where $|v| = \sum_{s \in v} |s|$. Let M_n^0, M_n^{12} and M_n^{123} be the numbers of elements with

length n in V_0 , V_{12} and V_{123} , respectively. It is easy to show that

$$\begin{aligned} M_n^0, M_n^{12} &\leq 2^{|s_1|+|s_2|+n} \\ M_n^{123} &\leq \sum_m 2^{|s_1|+|s_2|+m} 2^{\min\{m/2, (n-m)/6\}+(n-m)} \\ &\leq 7.2^{|s_1|+|s_2|+9n/8} \end{aligned}$$

and therefore

$$M_n \equiv M_n^0 + M_n^{12} + M_n^{123} \leq 9.2^{|s_1|+|s_2|+9n/8}. \quad (\text{A.8})$$

Moreover, if $L(s_1, s_2)$ denotes the distance of the supports of s_1 and s_2 , then

$$M_n = 0 \quad \text{for} \quad n < 2L(s_1, s_2) \quad (\text{A.10})$$

because every $v \in V_0 \cup V_{12} \cup V_{123}$ connects s_1 and s_2 with at least two chains of triangles. From (A.8)–(A.10) one finds

$$|\Delta(s_1, s_2)/T^2| \leq 9(1 - 2^{1/8}y)^{-1} (2/(1 - \varepsilon)^2)^{|s_1|+|s_2|} (2^{1/8}y)^{2L(s_1, s_2)}. \quad (\text{A.11})$$

Another trivial bound comes from I.19 and I.21:

$$|\Delta(s_1, s_2)/T^2| \leq 2(1 - \varepsilon)^{-|s_1|-|s_2|}. \quad (\text{A.12})$$

Now we are able to estimate $(TT_1 - U_1)/T^2$. Let η be some positive number; we get

$$\begin{aligned} (TT_1 - U_1)/T^2 &= \sum'_{(s_1, s_2): |s_1|+|s_2| < \eta\rho} \zeta^{s_1} \zeta^{s_2} \Delta(s_1, s_2)/T^2 \\ &\quad + \sum'_{(s_1, s_2): |s_1|+|s_2| \geq \eta\rho} \zeta^{s_1} \zeta^{s_2} \Delta(s_1, s_2)/T^2 \\ &= A_{<} + A_{>}. \end{aligned}$$

Using (A.3), (A.4) and (A.11) together with

$$L(s_1, s_2) \geq \rho - |s_1| - |s_2|$$

we find that

$$\begin{aligned} |A_{<}| &\leq a(x, \varepsilon) b(x, \varepsilon; \eta)^\rho \\ a(x, \varepsilon) &= 10.7(1 - \varepsilon - 2^{9/8}x)(1 - \varepsilon)^{-1}(1 - 2^{1/4}x)^{-1}x \\ b(x, \varepsilon; \eta) &= 2^{(9-\eta)/4}x^{2-\eta}(1 - \varepsilon)^{-2}. \end{aligned} \quad (\text{A.13})$$

To obtain a bound for $A_{>}$, we apply (A.3), (A.4) and (A.12). These give

$$|A_{>}| \leq 2(1 - y)^{-2} \eta \rho y^{\eta\rho}. \quad (\text{A.14})$$

Now we put

$$\begin{aligned} x &= 0.34 \\ \varepsilon &= 0.1 \end{aligned}$$

which were found to satisfy I.2, and choose η so that

$$b(x, \varepsilon; \eta) = (2x/(1 - \varepsilon))^\eta.$$

Substituting these values into equations (A.2), (A.5), (A.13) and (A.14) we obtain

$$\begin{aligned} |\langle \sigma^{d_1} \sigma^{d_2} \rangle_B - \langle \sigma^{d_1} \rangle_B \langle \sigma^{d_2} \rangle_B| &\leq |T_2/T| + |U_2/T^2| + |A_<| + |A_>| \\ &\leq 60\rho e^{-0.091\rho} < 10^6 \cdot e^{-0.09\rho} \end{aligned}$$

which is true for all B and therefore gives equation (9).

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