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Bounds on Ising partition functions I

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Abstract. The partition function Z of an Ising model can be considered as a polynomial of certain variables. The localization of the zeroes of this polynomial allows to determine the domain of analyticity of the free energy. We describe a new method which provides with domains where Z is not zero and permits to give bounds on Z and the correlation functions in these domains. Our method is expected to work particularly well in determining the high temperature domain of analyticity for Ising frustration models.

1. Introduction

Many of the rigorous methods to discuss the analytical properties of the free energy of statistical ensembles originate in the celebrated paper of Lee and Yang [1]. In their treatment, Lee and Yang considered the partition function of a ferromagnetic Ising model as a polynomial of $z = \exp(-2\beta h)$ where β is the inverse temperature and h is the external magnetic field. Basing on a theorem for polynomials of several complex variables (named 'circle theorem') they proved that all the zeroes of the partition function lie on the unit circle, $|z| = 1$. This implied the analyticity of the free energy for real non-zero values of h . Perhaps the most successful extension of this method was due to Asano [2] and Ruelle [3]. Here again, the starting point was a so called 'Contraction theorem' on polynomials by which the zeroes of the partition functions of models with non-ferromagnetic interactions could be localized and bounds on the domain of analyticity of the free energy were obtained (see, e.g., Sarbach and Rys [4] and Gruber et al. [5]).

This work, presented in two papers, is intended to provide with a powerful Lee-Yang type method for discussing the analytical behaviour of the free energy and the correlations in the so called frustration models. In these models, the different interactions compete with each other as to their effect on the orientation of the spins. The consequences of this competition are, perhaps, the most interesting in the case of Ising spins: these may become 'frustrated', not being able to 'decide' which orientation to take up. As a result, one may find a multiple degeneracy of the minimum energy level: the number of ground states may go to infinity with the increasing volume. This is in contrast with the ferromagnetic and

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other non-frustrated Ising models, where the ground state degeneracy follows from the symmetry of the Hamiltonian and is, therefore, finite.

The necessity for the elaboration of a new method is explained by this difference. The technique of Asano contraction applies also to Ising frustration models. However, the best estimate for the domain of analyticity, attainable by the Asano contraction, is obtained for ferromagnets in external field; namely, one can reproduce Lee and Yang's result. The physical reason for the absence of second order phase transitions in this latter case is the uniqueness of the ground state. (This might allow first order transitions, which do not occur, either.) At any finite temperature the system is magnetized and therefore one may say that the critical temperature is $T_c = +\infty$. Now in frustration models, at zero temperature there are still infinitely many available spin configurations, which is a typical high temperature (H.T.) situation: the frustration 'heats up' the system. If in such a model there is no phase transition, the system is certainly above its critical point at any positive temperature; the critical temperature may then be considered as $T_c = 0$.

In technical terms, the Asano contraction gives the best results in estimating the low temperature (L.T.) domain (below T_c) of analyticity of the free energy. For treating the problem of frustration, we need another method which is the best if one applies it to estimate the H.T. domain (above T_c) of analyticity.

Similarly to the authors mentioned earlier, we consider the partition function of an Ising model as a polynomial of the variables $\tanh \beta J_b$ (H.T. situation) or $\exp(-2\beta J_b)$ (L.T. situation), where J_b is the strength of the bond b . In both cases, this polynomial is linear in each of the variables and any of its additive terms can be assigned to a set of bonds. These sets form a group, which is called the H.T. and L.T. Group, respectively (see [5]). Both groups are embedded in a larger group which is formed by all subsets of the total family of bonds. In Section 2, we therefore study polynomials, the structure of which corresponds to the above description. In a certain domain of the variables we give upper and lower bounds on the absolute value of these polynomials. The lower bound being positive, the zeroes of the polynomial are outside this domain: that is the property needed to prove the analyticity of the free energy. In Section 3 we establish the formal connection between the polynomials of Section 2 and the Ising partition functions and correlations. Our method, though aimed to discuss frustration models, is applicable to reproduce different results on high and low temperature analyticity in general Ising models. This possibility is briefly considered in Section 4. Finally, in Section 5 we summarize the results from the point of view of future applications.

2. Bounds on polynomials

We are going to consider polynomials of K complex variables, z_1, \dots, z_K . Let $Q = \{1, 2, \dots, K\}$ and $P(Q)$ denote the set of all subsets of Q . We make use of two properties of $P(Q)$.

(i) $P(Q)$ is partially ordered w.r.t. the inclusion: if a_1 and a_2 are subsets of Q , then a_1 is smaller than a_2 if $a_1 \subset a_2$. For any $A = \{a_1, \dots, a_n\}$, where $a_i \subset Q$, let $\inf A$ denote the minimal elements of $A - \{\emptyset\}$; i.e., $a_i \in \inf A$ means that no element of A is included in a_i , except a_i itself and, possibly, the empty set. If A has elements different from the empty set, then $\inf A$ is not empty.

(ii) $P(Q)$ is a group w.r.t. the symmetric difference of its elements: if g_1 and g_2 are parts of Q then

$$g_1 g_2 = (g_1 \cup g_2) - (g_1 \cap g_2)$$

is their symmetric difference.

Now let G be a subgroup of $P(Q)$ such that it is uniquely generated by $\inf G$ in the following sense: for any $g \in G$ there is a unique set

$$\{g_1, \dots, g_k\} \subset \inf G$$

such that

$$g_i \cap g_j = \emptyset \quad \text{if } i \neq j$$

and

$$g = g_1 \cup \dots \cup g_k.$$

For any $i \in Q$ let $N_n(i)$ be the number of those elements of $\inf G$ which contain i and exactly $n-1$ other points of Q . For any $n > 0$ we choose a number $N_n \geq N_n(i)$. Now the following statement is true.

Lemma 1. Consider the polynomial

$$R(z) = \sum_{g \in G} \prod_{i \in g} z_i \equiv \sum_{g \in G} z^g \quad (1)$$

and suppose that

$$\sum_{n>0} N_n x^n / (1-\varepsilon)^{n-1} \leq \varepsilon \quad (2)$$

is satisfied by some $x > 0$ and $\varepsilon < 1$. Then

$$(1-\varepsilon)^K \leq |R(z)| \leq (1+\varepsilon)^K$$

if $|z_i| \leq x$ for all $i \in Q$.

Proof. For any $\alpha \subset Q$ let

$$G_\alpha = \{g \in G : g \subset \alpha\}$$

$$R_\alpha = \sum_{g \in G_\alpha} z^g \quad (3)$$

$$r_\alpha^i = \sum_{i \in g \in G_{\alpha \cup \{i\}}} z^g / R_\alpha$$

and

$$[i] = \{1, \dots, i\}. \quad (4)$$

We have the following product representation of R .

$$\begin{aligned} R &= R_{[K-1]}(1 + r_{[K-1]}^K) \\ &= R_{[K-2]}(1 + r_{[K-2]}^{K-1})(1 + r_{[K-1]}^K) \\ &= \dots = \prod_{i=1}^K (1 + r_{[i-1]}^i) \end{aligned} \quad (5)$$

The proof can be performed by showing that $|r_\alpha^i| \leq \varepsilon$ for any $i \in Q$ and $\alpha \subset Q$, provided that $|z_j| \leq x$ for any $j \in Q$. We do this by induction according to $|\alpha|$, the number of points in α . For $\alpha = \emptyset$ we have

$$r_\emptyset^i = \begin{cases} z_i & \text{if } \{i\} \in G \\ 0 & \text{otherwise.} \end{cases}$$

Therefore,

$$|r_\emptyset^i| \leq x = N_1 x \leq \sum_n N_n x^n / (1 - \varepsilon)^{n-1} \leq \varepsilon.$$

Suppose now that $|r_\alpha^j| \leq \varepsilon$ is proved for any j and α with $|\alpha| < i$. It is sufficient to show that $|r_{[i]}^{i+1}| \leq \varepsilon$; for other sets we get the result by permutation. Now

$$r_{[i]}^{i+1} = \sum_{i+1 \in g \in \inf G_{[i+1]}} z^g R_{[i]-g} / R_{[i]} \quad (6)$$

where we used that g has a unique decomposition into the disjoint union of the elements of $\inf G$. On the other hand, if

$$g = \{i+1, j_2, \dots, j_n\} \subset [i+1]$$

and

$$g'k = \{j_2, \dots, j_k\}$$

then

$$R_{[i]} = R_{[i]-g} \prod_{k=2}^{|g|} (1 + r_{[i]-g'k}^{j_k}) \quad (7)$$

where $|g| = \text{card } g = n$. Putting (7) into (6) one obtains

$$r_{[i]}^{i+1} = \sum_{i+1 \in g \in \inf G_{[i+1]}} z^g / \prod_{k=2}^{|g|} (1 + r_{[i]-g'k}^{j_k}) \quad (8)$$

For each r_α^j in the denominator α has at most $i-1$ points and therefore r_α^j is bounded by ε . Then equations (8) and (2) clearly imply that $r_{[i]}^{i+1}$ is bounded by ε . \square

In the following, we discuss a possibility to obtain bounds on the polynomial R of equation (1), even if G is not uniquely generated by $\inf G$.

Let $\{Q^i\}_{i=1, \dots, N}$ be a disjoint cover of Q :

$$Q = \bigcup_{i=1}^N Q^i \quad \text{and} \quad Q^i \cap Q^j = \emptyset \quad \text{if } i \neq j.$$

Let G^0 be a subgroup of G , defined by

$$G^0 = \{g \in G : g \cap Q^i \in G \text{ for any } i\} \quad (9)$$

Consider the quotient group, G/G^0 . We show that under certain conditions it may substitute G in Lemma 1. Let

$$G^i = \{g \in G : g \subset Q^i\}$$

then, clearly, G^i is a subgroup of G^0 and also it is the projection of G^0 into Q^i . In general, if A is a coset of G according to G^0 then

$$\text{Proj}_i A = \{g \cap Q^i : g \in A\} \quad (10)$$

is a coset of $P(Q^i)$ – the power set of Q^i – according to G^i . Any $A \in G/G^0$ is uniquely represented by the set of those projections (10) which differ from the corresponding G^i : if

$$a^m = \text{Proj}_m A \begin{cases} \neq G^m & \text{for } m = i_1, \dots, i_k \\ = G^m & \text{otherwise} \end{cases} \quad (11a)$$

then this set is

$$s_A = \{a^{i_1}, \dots, a^{i_k}\} \quad (11b)$$

Now let

$$\hat{Q} = \bigcup_{i=1}^N \hat{Q}^i$$

where

$$\hat{Q}^i = (P(Q^i)/G^i) - G^i$$

and let

$$S = \{s \subset \hat{Q} : s = s_A \text{ for some } A \in G/G^0\} \quad (12)$$

Clearly, if $s \in S$ then $\text{card}(s \cap \hat{Q}^i) \leq 1$ for any i . The elements of S form a group: if $s, s' \in S$ then $s = s_A, s' = s_B$ for some $A, B \in G/G^0$; let now

$$\text{Proj}_i A = a^i \quad \text{and} \quad \text{Proj}_i B = b^i$$

then

$$ss' = \{a^i b^i\}_{i=1}^N - \{G^i\}_{i=1}^N \in S$$

defines the group operation. Here

$$a^i b^i = \{gg' \subset Q^i : g \in a^i, g' \in b^i\}$$

is a coset of $P(Q^i)$. The group S is isomorphic with G/G^0 . S is ordered w.r.t. the inclusion and $\inf S$ is the set of the minimal elements of $S - \{\emptyset\}$; $\inf G/G^0$ is that part of G/G^0 which is isomorphic with $\inf S$.

The cover of Q can always be chosen so that $\inf S$ uniquely generates S , in the sense we used it earlier (indeed, for instance, covers with at most three subsets all have this property). This can be told as $\inf G/G^0$ uniquely generates G/G^0 . To G^0 , one can assign a polynomial analogous to (1):

$$R^0(z) = \sum_{g \in G^0} z^g = \prod_{i=1}^N \sum_{g \in G^i} z^g \quad (13)$$

Now one obtains the following result.

Lemma 2. Let $Q = \{1, \dots, K\}$, G be the subgroup of $P(Q)$ and a cover $\{Q^i\}_{i=1, \dots, N}$ be given so that, with G^0 defined by (9), $\inf G/G^0$ uniquely generates G/G^0 . Let, moreover

$$N_n(i) = \text{card} \{A \in \inf G/G^0 : \text{Proj}_k A \neq G^k \text{ for } k = i \text{ and for exactly } n-1 \text{ other values of } k\} \quad (14)$$

and N_n be chosen so that

$$N_n \geq N_n(i) \quad \text{for } i = 1, \dots, N \quad (15)$$

Suppose that (2) holds with these N_n and with some $x > 0$ and $\varepsilon < 1$. Let R and R^0 be the polynomials defined in (1) and (13), respectively. Then

$$(1 - \varepsilon)^{N-1} \leq |R(z)/R^0(z)| \leq (1 + \varepsilon)^{N-1} \quad (16)$$

provided that

$$\left| \sum_{g \in a^i} z^g / \sum_{g \in G^i} z^g \right| \leq x$$

for any $1 \leq i \leq N$ and $a^i \in \hat{Q}^i$.

Proof. Let S be the group (12) and for any $a \in \hat{Q}$, let ζ_a be a complex variable assigned to a . Consider the polynomial

$$T(\zeta) = \sum_{s \in S} \prod_{a \in s} \zeta_a \equiv \sum_{s \in S} \zeta^s \quad (17a)$$

It is easy to show that

$$T(\zeta) = R(z)/R^0(z) \quad (17b)$$

if, for any $i = 1, \dots, N$ and $a^i \in \hat{Q}^i$, one makes the substitution

$$\zeta_{a^i} = \sum_{g \in a^i} z^g / \sum_{g \in G^i} z^g \quad (17c)$$

Hence, one has to prove only that the bounds (16) are valid for $T(\zeta)$ if $|\zeta_a| \leq x$ for any $a \in \hat{Q}$. We introduce the following notations: let $\alpha \subset \{1, \dots, N\}$, then

$$\begin{aligned} S_\alpha &= \left\{ s \in S : s \subset \bigcup_{i \in \alpha} \hat{Q}^i \right\} \\ \mathbf{s} &= \{i \in \{1, \dots, N\} : s \cap \hat{Q}^i \neq \emptyset\} \\ T_\alpha &= \sum_{s \in S_\alpha} \zeta^s \\ t_\alpha^i &= \sum_{s \in S_{\alpha \cup \{i\}}; i \in \mathbf{s}} \zeta^s / T_\alpha \end{aligned} \quad (18)$$

The equations (18) are analogous to equations (3), just as

$$T = \prod_{i=1}^{N-1} (1 + t_{[i]}^{i+1}) \quad (19)$$

and

$$t_{[i]}^{i+1} = \sum_{s \in \inf S_{[i+1]}; i+1 \in \mathbf{s}} \zeta^s / \prod_{k=2}^{|\mathbf{s}|} (1 + t_{[i]-s'k}^{j_k}) \quad (20)$$

are analogues of equations (5) and (8), respectively. In (20), j_k is the k th point of

$$\mathbf{s} = \{i+1, j_2, \dots, j_n\}$$

and

$$s'k = \{j_2, \dots, j_k\};$$

the cardinals of s and \mathbf{s} are the same: $|s| = |\mathbf{s}|$. Noticing that

$$N_n(i) = \text{card} \{s \in \inf S : |s| = n \text{ and } s \cap \hat{Q}^i \neq \emptyset\}$$

one can conclude the proof by showing, in the same way as in Lemma 1, that

$$|t_\alpha^i(\zeta)| \leq \varepsilon \quad (21)$$

for any $1 \leq i \leq N$, $\alpha \in \{1, \dots, N\}$. \square

So far, we considered only the subgroup G of $P(Q)$; now for any $D \in P(Q)/G$, one can define

$$R^D(z) = \sum_{g \in D} z^g$$

In view of applications, it is interesting to obtain bounds also on R^D/R . To this end, let us continue the earlier discussion. In fact, G^0 of equation (9) factorizes not only G but also the whole $P(Q)$. Meanwhile, it factorizes the elements of $P(Q)/G$ distinctly. For $D \in P(Q)/G$, let

$$D/G^0 = \{A \in P(Q)/G^0 : A \subset D\}.$$

Now we extend the definition of s_A , as given in equations (10), (11), to any $A \in P(Q)/G^0$ and consider the set

$$S^D = \{s \subset \hat{Q} : s = s_A \text{ for some } A \in D/G^0\}$$

A polynomial

$$T^D(\zeta) = \sum_{s \in S^D} \zeta^s$$

can be assigned to S^D ; it is easy to show that

$$T^D(\zeta) = R^D(z)/R^0(z) \quad (22)$$

if ζ is given by equation (17c). Equation (22) is a generalization of (17b); for $D = G$ the two equations coincide. Dividing (22) by (17b) one obtains

$$R^D(z)/R(z) = T^D(\zeta)/T(\zeta) \quad (23)$$

For $D \in (P(Q)/G) - G$, let $\inf S^D$ denote the set of minimal elements of S^D . Any $s \in S^D$ can be written as

$$\begin{aligned} s &= s_1 \cup s_2 \\ s_1 \cap s_2 &= \emptyset \\ s_1 &\in \inf S^D, \quad s_2 \in S \end{aligned} \quad (24)$$

though, in general, this decomposition is not unique. The cover of Q can always be chosen so that $\inf G/G^0$ uniquely generates G/G^0 and also, the decomposition (24) is unique for any $D \in (P(Q)/G) - G$ and $s \in D$. (This is true, for example, for the trivial cover $\{Q\}$ and the cover with two disjoint sets $\{Q^1, Q^2\}$.) Assume that the cover, we have chosen to Lemma 2, satisfies these conditions. Then we can write

$$T^D(\zeta)/T(\zeta) = \sum_{s \in \inf S^D} \zeta^s T_{[N]-s}/T_{[N]}$$

where we applied the notations (4) and (18) (notice that $T_{[N]} = T$). The analogue of equation (7) gives then

$$T^D(\zeta)/T(\zeta) = \sum_{s \in \inf S^D} \zeta^s / \prod_{k=1}^{|s|} (1 + t_{[N]-s'k}^{j_k}) \quad (25)$$

Let now

$$N_n^D = \text{card} \{s \in \inf S^D : |s| = n\} \quad (26)$$

From equations (21), (23), (25) and (26) we find

$$|R^D(z)/R(z)| \leq \sum_n N_n^D x^n / (1 - \varepsilon)^n \quad (27)$$

provided that $|\zeta_{a^i}| \leq x$ for any ζ_{a^i} , given by (17c).

3. Bounds on Ising partition functions and correlations

The results of the former section can be applied to study Ising models. Let \mathbb{Z} be a lattice and $\sigma : \mathbb{Z} \rightarrow \pm 1$ be a spin configuration. The potential of a finite subsystem of spins is defined as

$$H_B(\sigma) = - \sum_{b \in B} J_b \prod_{x \in b} \sigma(x) \equiv - \sum_{b \in B} J_b \sigma^b \quad (28)$$

where B is a finite family of finite subsets of \mathbb{Z} . Now H_B defines the probability distribution of the spins on

$$\Lambda = \bigcup_{b \in B} b$$

and the corresponding partition function can be written as

$$Z_B = \sum_{\sigma|_\Lambda} \exp(-\beta H_B(\sigma)) = 2^{|\Lambda|} \left(\prod_{b \in B} \cosh \beta J_b \right) R$$

Here R is defined by the H.T. expansion as

$$R = \sum_{g \in G} \prod_{b \in g} \tanh \beta J_b \quad (29)$$

and G is the 'High Temperature Group' [5]:

$$(b_1, \dots, b_k) \in G$$

if and only if $b_i \in B$ and $b_1 b_2 \cdots b_k = \emptyset$ ($bc = (b \cup c) - (b \cap c)$). Now R can play the role of the polynomial (1) if one identifies the set of bonds B with the set Q and the complex variables z_i , $i \in Q$, with

$$z_b = \tanh \beta J_b, \quad b \in B. \quad (30)$$

Furthermore, if $D \in P(Q)/G$, then there is a $d \subset \Lambda$ such that

$$\prod_{b \in g} b = d$$

for any $g \in D$: the cosets can be indexed with the subsets of the lattice. Now if

$$R^d = \sum_{g \in D} \prod_{b \in g} \tanh \beta J_b$$

then

$$R^d/R = \langle \sigma^d \rangle_B$$

where $\langle \cdot \rangle_B$ denotes the mean value according to the probability distribution defined by the potential (28). The bound (27) then refers to $\langle \sigma^d \rangle_B$. The variables, introduced in (17c), also correspond to correlations: let $B^i \subset B$ and $G^i = G \cap P(B^i)$. The cosets of $P(B^i)$, according to G^i , can also be indexed with the subsets of

$$\Lambda^i = \bigcup_{b \in B^i} b.$$

Let $b \subset \Lambda^i$ correspond to $a \in P(B^i)/G^i$; then

$$\zeta_a = \langle \sigma^b \rangle_{B^i} \quad (31)$$

where the mean value is taken according to the probability distribution

$$\sim \exp(-\beta H_{B^i}(\sigma)) = \exp\left(\beta \sum_{b \in B^i} J_b \sigma^b\right).$$

If $\{B^i\}_{i=1}^N$ is a partition of B and G^0 and $\{G^i\}_{i=1}^N$ are the subgroups of G corresponding to this partition, then by using equations (13), (17) and (30) we obtain

$$Z_B = 2^{|\Lambda|} \left\{ \prod_{i=1}^N \left(\prod_{b \in B^i} \cosh \beta J_b \right) \left(\sum_{g \in G^i} \prod_{b \in g} \tanh \beta J_b \right) \right\} T(\zeta) \quad (32)$$

The prefactor of T in this equation is the partition function of the union of independent small subsystems. If, while taking the thermodynamic limit, the sets B^i are kept to be small (i.e., the number of bonds in B^i is bounded while i goes to infinity) then the possible singularities of the free energy come from the zeroes of $T(\zeta)$. In fact, the sum (17a) which defines $T(\zeta)$ can be considered as a high temperature expansion where the 'small variables' are the ζ_a 's of equation (31), instead of $\tanh \beta J_b$, the 'small variables' of the usual H.T. expansion.

4. A remark on the high and low temperature analyticity

Another variation of Lemma 1, if applied to the high and low temperature groups (see [5]), can be used to show high and low temperature analyticity properties of Ising models with any kind of finite range interactions. To obtain these results, let us consider the set of lattice sites Λ and that of the bonds, B . We choose a cover $\{B^i\}_{i \in \Lambda}$ for B so that B^i includes all the bonds containing the site i . Now $\text{con } G$ denotes the set of the connected elements of G , where G is either the high or the low temperature group. That is, if $g \in \text{con } G$ then the bonds of g cover a connected set of sites in Λ . Clearly, there is a unique way to write any $g \in G$ as the disjoint union of connected elements. By substituting $\text{inf } G$ with $\text{con } G$ in the

definition of $N_n(i)$ and by modifying r_α^i in an obvious way, one obtains exponential upper and lower bounds on the absolute value of the partition function provided that $|\tanh \beta J_b|$ or $|\exp(-\beta |J_b|)|$ are small enough. Then the analyticity of the free energy can be proved by Vitali's convergence theorem [6]. We remark that the low temperature analyticity can be shown only for non-frustrated models. In this way, we can merely reproduce earlier results (e.g., some of Gruber et al., [5]); therefore, we do not discuss this possibility in detail.

5. Summary

In this paper we developed a new method for the localization of the zeroes of Ising partition functions. We emphasize two particular features of our method, which affect the future applications. First, beside determining domains where the partition function, Z , is not zero, we obtain estimates on $|Z|$ and also on the correlation functions in the same domain (cf. equation (27)). Second, our results strongly depend on the lattice structure and the range of interaction through the quantities $N_n(i)$, of equation (14). This is in contrast with Lee and Yang's finding for ferromagnetic models. This structure dependence may somewhat be exaggerated, because our method does not take into account a possible compensation among terms of different signs in the polynomial (1); nevertheless, it may reflect an existing feature of the distribution of the zeroes. Regarding the applications, a consequence of this structure dependence is that one needs estimates of the lattice-combinatorial quantities $N_n(i)$, as good as possible.

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